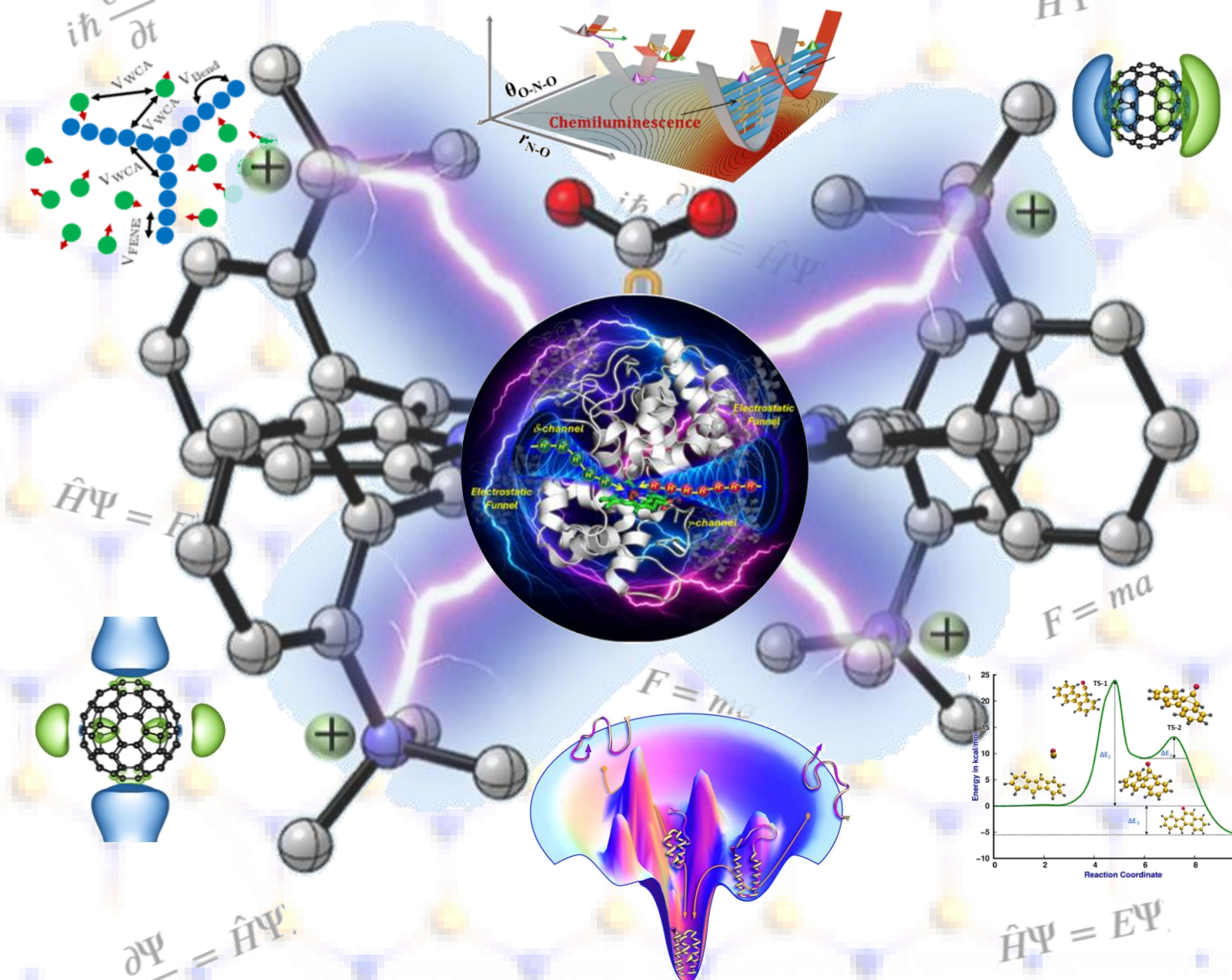
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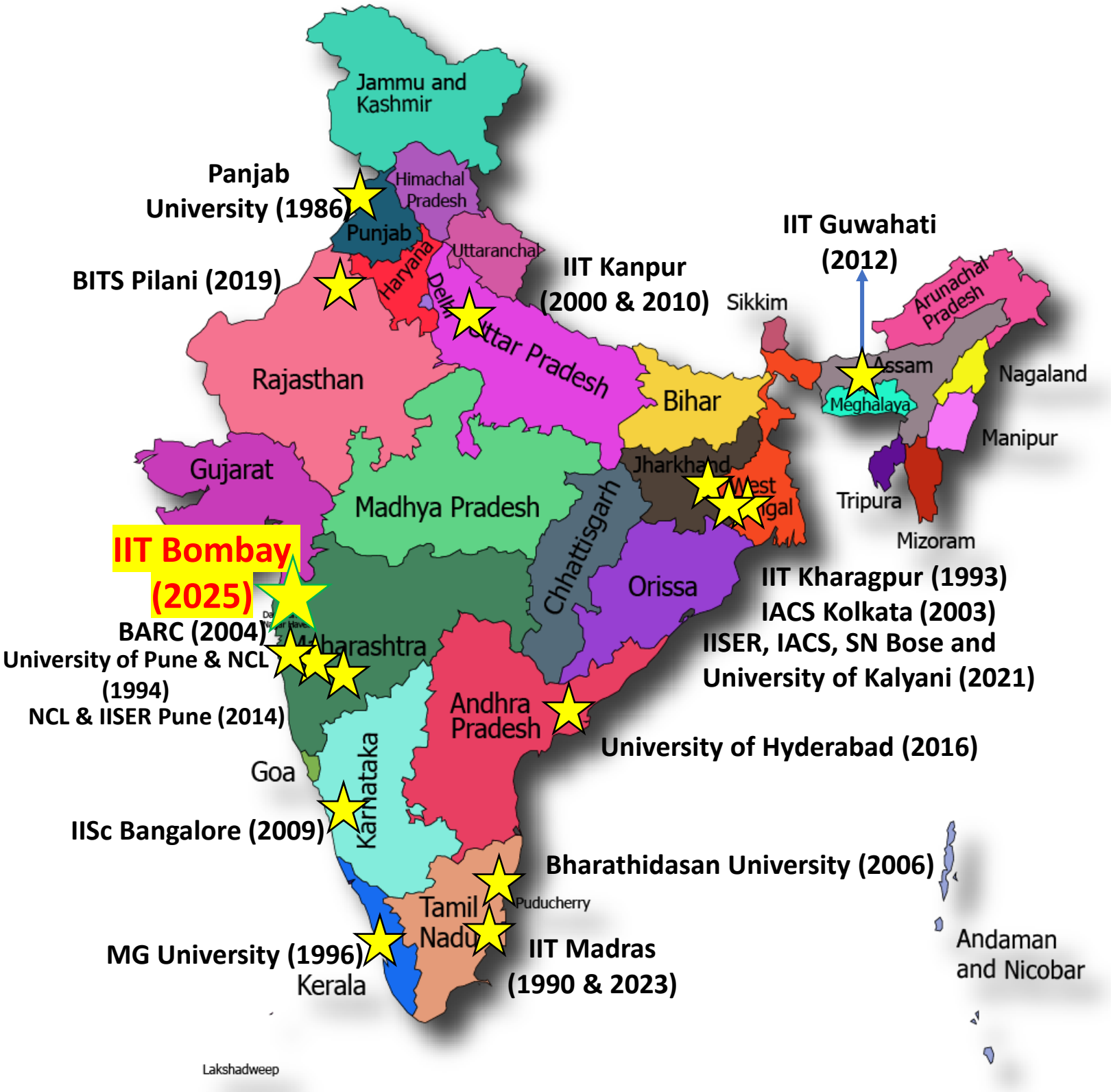
Theoretical Chemistry Symposium 2025

2-5 December, 2025

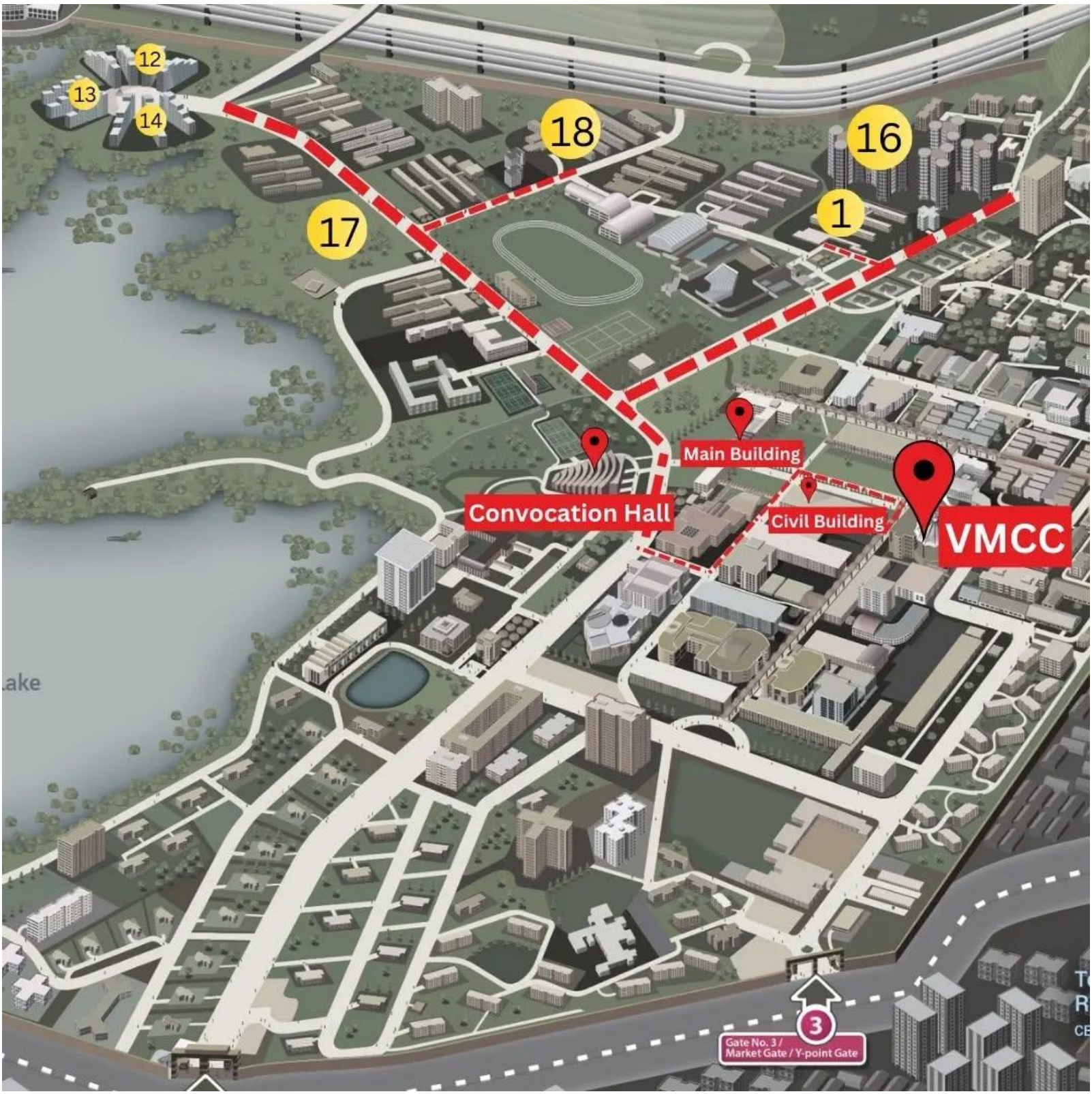


Department of Chemistry
Indian Institute of Technology Bombay
Powai, Mumbai, 400076

TCS So far ...


Jammu and Kashmir
Panjab University (1986)
Himachal Pradesh
Punjab
Uttaranchal
Haryana
BITS Pilani (2019)
IIT Kanpur (2000 & 2010)
IIT Guwahati (2012)
Sikkim
Arunachal Pradesh
Assam
Nagaland
Meghalaya
Manipur
Tripura
Mizoram
Rajasthan
Uttar Pradesh
Bihar
Jharkhand
West Bengal
Gujarat
Madhya Pradesh
Chhattisgarh
Orissa
IIT Bombay (2025)
BARC (2004)
University of Pune & NCL (1994)
NCL & IISER Pune (2014)
IIT Kharagpur (1993)
IACS Kolkata (2003)
IISER, IACS, SN Bose and University of Kalyani (2021)
Maharashtra
Andhra Pradesh
University of Hyderabad (2016)
Goa
Karnataka
IISc Bangalore (2009)
Bharathidasan University (2006)
Puducherry
Tamil Nadu
MG University (1996)
Kerala
IIT Madras (1990 & 2023)
Andaman and Nicobar
Lakshadweep

Theoretical Chemistry Symposium 2025



Indian Institute of Technology Bombay
भारतीय प्रौद्योगिकी संस्थान
मुंबई

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Web: www.iitb.ac.in

19th Theoretical Chemistry Symposium (TCS 2025) Schedule

Day 1	2nd December 2025			Day 2 - 4	3rd December 2025			4th December 2025			5th December 2025		
08:00-09:00 AM	Registration			Session 1	*B. Nag Auditorium*			*B. Nag Auditorium*			*B. Nag Auditorium*		
09:00-10:00 AM	*B. Nag Auditorium*			09:00-09:45 AM	SC10: Biman Bagchi			SC22:Sourav Pal			SC34: Satrajit Adhikari		
	Inauguration				PL4: Raghavan B. Sunoj (IITB)			PL6: Balasubramanian Sundaram (JNCASR)			PL8: Graham Worth (UCL)		
Session 1	*B. Nag Auditorium*			Session 2	*Room 21*	*Room 22*	*Room 23*	*Room 21*	*Room 22*	*Room 23*	*Room 21*	*Room 22*	*Room 23*
	SC1: Eluvathingal D. Jemmis				SC11: Debayan Chakraborty	SC12: Ayan Datta	SC13: Arun K Manna	SC23: Kumar Vanka	SC24: L. Senthilkumar	SC25: Madhurima Jana	SC35: Parameswaran Pattiyil	SC36: Pattath D. Pancharatna	SC37: Ponnambalam Venuvanalingam
10:00-10:45 AM	PL1: Keshavamurthy Srihari (IITK)			9:50-10:10 AM	IL19: Konstantinos D. Vogiatzis	IL20: Anik Sen	IL21: Peter Comba	IL49: Michael Klein	IL50:Upendra Harbola	IL51: Michal Repisky	IL79: Prashant Manohar	IL80: Puneet Gupta	IL81: Hemant K. Kashyap
				10:10-10:30 AM	IL22: Anatoly Kolomeisky	IL23: K. V. Jovan Jose	IL24: Pradipta Bandyopadhyay	IL52: G. Narahari Sastry	IL53: Divya Nayar	IL54: Sudip Chakraborty (CUP Punjab)	IL82: Srinivasu Kancharlapalli	IL83: Shivnath Mazumder	IL84: Pralok Kumar Samanta
10:45-11:30 AM	PL2: Joan-Emma Shea (UC, Santa Barbara)			10:30-10:50 AM	IL25: Dmitrii E. Makarov	IL26: Upakarasamy Lourderaj	IL27: Saurabh Kumar Singh	IL55: Susanta Mahapatra	IL56: Soumen Ghosh	IL57: Anirban Mondal	IL85: Raghunathan Ramakrishnan	IL86: Vamsee Voora	IL87: Nisanth N. Nair
				10:50-11:10 AM	IL28: Pushpita Ghosh	IL29: Venkatesan Subramanian	IL30: HPE Bibhu Dash	IL58: Martin Srnec	IL59: Priyadarshi Satpati	IL60: Prabha Vadivelu	IL88: Jayashree Nagesh	IL89: Shubhra Ghosh Dastidar	IL90: Ravi Venkatramani
Tea Break (11:30-11:50 AM)				Tea Break (11:10-11:30 AM)*									
Session 2	*Room 21*	*Room 22*	*Room 23*	Session 3	*Room 21*	*Room 22*	*Room 23*	*Room 21*	*Room 22*	*Room 23*	*Room 21*	*Room 22*	*Room 23*
	SC2: Abhishek Sirohiwal	SC3: Mahesh Sundararajan	SC4: Balanarayan Pananghat		SC14: Arnab Ghosh	SC15: Prasad L. V. K. Dasari	SC16: Debashree Chakraborty	SC26: Aryya Ghosh	SC27: Mahesh Gudem	SC28: Manoj K. Mishra	SC38: Amrita Bhattacharya	SC39: Rudraditya Sarkar	SC40: Niharendu Chaudhary
11:50 AM-12:10 PM	IL1: Deva Priyakumar U	IL2: Arnab Bhattacherjee	IL3: Alexey A. Popov	11:30-11:50 AM	IL31: Dimitrios A. Pantazis	IL32: Kaushik Talukdar	IL33: Paranjothy Manikandan	IL61: Federico Totti	IL62: Sudip Chakraborty (HRI Allahabad)	IL63: Deepa Janardanan	IL91: Padmesh Anjukandi	IL92: Alessandro Soncini	IL93: Suman Chakrabarty
12:10-12:30 PM	IL4: Kalisankar Bhattacharyya	IL5: Susmita De	IL6: Rukmankesh Mehra	11:50 AM-12:10 PM	IL34: Nico van der Vegt	IL35: Raja Ghosh	IL36: Muthukumar Kaliappan	IL64: Andrew M. Rappe	IL65: Avisek Das	IL66: Prakash Muthuramalingam	IL94: Sangita Sen	IL95: Yesodharan Sajeev	IL96: Sanjay Kumar
12:30-12:50 PM	IL7: Sai Ganesh Ramesh	IL8: Mudit Dixit	IL9: Jagannath Mondal	12:10-12:30 PM	IL37: Ankan Paul	IL38: John McGrady	IL39: AMD Sudhakar Yerneni	IL67: Pinku Nath	IL68: Md. Mehboob Alam	IL69: Govardhan Reddy	IL97: Sandeep Kumar	IL98: Nicholas T Bronn	IL99: Rajeev Ramanan
12:50-1:10 PM	SOP1: Imon Mandal/ 2: Sruthi Sudhakar	SOP3: Ankita Narwal/ 4: Nandu P S	SOP5: Dyuti Chatterjee / 6: Prashant Kumar	12:30-12:50 PM	SOP13: Thakur Rochak Kumar Rana/ 14: Sheetal Ranaut	SOP15: Ritwika Dey/ 16: Akhilesh Sharma	SOP17: Sougata Saha/ 18: Nikhitha R.	SOP25: Ritesh Goutam Nayak/ 26: Rinu Jacob	SOP27: Devansh Sharma/ 28: Shym Sharan Tripathi	SOP29: Rajalakshmi C/ 30: Shamik Chanda	IL100: Vidya Avasare	IL101: AMAT Gopi Chandran	IL102: Wiley Partha Pratim Pal
											Closing Ceremony and Prize Distribution (*B. Nag Auditorium)* 12:50-1:20 PM		
Lunch Break (1:10-2:00 PM)				Lunch Break (12:50-1:40 PM)							Lunch Break (1:20-2:10 PM)		
Session 3	*B. Nag Auditorium*			Session 4	*B. Nag Auditorium*			*B. Nag Auditorium*					
	SC5: Shridhar R. Gadre				SC17: Swapan Kumar Ghosh			SC29: Suryanarayana Ramasesha					
2:00-2:45 PM	PL3: Andreas Dreuw (UH)			1:40-2:25 PM	PL5: Parbati Biswas (DU)			PL7: Martin Head-Gordon (UC, Berkeley)					
Session 4	*Room 21*	*Room 22*	*Room 23*	Session 5	*Room 21*	*Room 22*	*Room 23*	*Room 21*	*Room 22*	*Room 23*			
	SC6: Snehasis Daschakraborty	SC7: Ambar Banerjee	SC8: Kalidas Sen		SC18: Srabanti Chaudhury	SC19: Sambhu N. Datta	SC20: K. Senthilkumar	SC30: Y. U. Sasidhar	SC31: Biswarup Pathak	SC32: R. S. Swathi			
2:50-3:10 PM	IL10: Jer-Lai Kuo	IL11: Bidisa Das	IL12: Anirban Misra	2:30-2:50 PM	IL40: Neetu Goel	IL41: Balamurugan Kanagasabai	IL42: Amartya Bose	IL70: Anoop Ayyappan	IL71: Raghunath O. Ramabhadran	IL72: Debasish Mondal			
3:10-3:30PM	IL13: Kousik Samanta	IL14: Bhaskar Mondal	IL15: Swapan K Pati	2:50-3:10 PM	IL43: Rakesh Singh	IL44: Nayana Vaval	IL45: Azaj Ansari	IL73: Charulatha Venkataraman	IL74: Somrita Ray	IL75: Pallavi Debnath			
3:30-3:50 PM	IL16: Ram Kinkar Roy	IL17: Susmita Roy	IL18: Prabhat K. Sahu	3:10-3:30 PM	IL46: Tarak Karmakar	IL47: NVIDIA Manish Modani	IL48: Rajib Biswas	IL76: Niladri Patra	IL77: Amit Kumar Paul	IL78: Biman Jana			
3:50-4:10 PM	SOP7: Sisodiya Dilawar Singh/ 8: Aanchal Grover	SOP9: Vaibhav Bhatt/ 10: Atreyee Majumdar	SOP11: Tanwi Debnath/ 12:Gargee Kashyap	3:30-3:50 PM	SOP19: Bitap Raj Thakuria/ 20: Shreya Verma	SOP21: Arup Sarkar/ 22: George Devasia	SOP23: Nayana E C/ 24: Shalini Yadav	SOP31: Vipanchi/ 32: Bhawna	SOP33: Rounak Nath/ 34: Chandraniv Dey	SOP35: Arzoo Rai / 36: Samir Kumar Nayak			
Tea Break (4:10-4:30 PM)				Tea Break (3:50-4:10 PM)									
Session 5	SC9: K. R. S. Chandrakumar, Jaccob Madhavan, Vignesh Kuduva R, Asis Jana			Session 6	SC21: Sailaja Krishnamurty, Ranganathan Subramanian, Musharaf Ali Sheikh, Debasis Koley, Mahesh K. Ravva, Rahul Shukla			SC33: T. J. Dhilip Kumar, Tammineni Rajagopala Rao, Tapta Kanchan Roy, Nidhi Malhotra, C. N. Ramachandran					
4:30-6:30 PM	Poster Session			4:10-6:00 PM	Poster Session			Poster Session					
7:00-8:00 PM	Dinner			6:00-8:00 PM	Cultural Programme# and Dinner			Gala Dinner					

PL = Plenary Lectures (8 x 45 min)

IL = Invited Lectures (102 x 20 min)

SOP = Short Oral Presentation (36x10 min)

*Photo Session (3rd Dec 2025)

#P.C. Saxena Auditorium (6:00 to 7:00 PM)

Sponsors Talk

Preface

On behalf of the Organising Committee, it is our pleasure to welcome you to the 19th Theoretical Chemistry Symposium (TCS-2025), hosted by the Department of Chemistry, Indian Institute of Technology Bombay, at the Victor Menezes Convention Centre (VMCC), Mumbai, during 2–5 December 2025. The Theoretical Chemistry Symposium, first held in 1986 at Panjab University, Chandigarh, has since been organized across leading institutions including IIT Madras, IIT Kharagpur, University of Pune and NCL, M.G. University, University of Hyderabad, IIT Kanpur, IACS Kolkata, BARC Mumbai, Bharathidasan University, IISc Bangalore, IIT Guwahati, IISER Pune, BITS Pilani, IISER Kolkata, and IIT Madras in 2023. Over the years, eminent theoreticians such as A. B. Sannigrahi, A. Chandra, B. Bagchi, D. Mukherjee, E. D. Jemmis, K. D. Sen, K. L. Sebastian, M. Durgaprasad, M. S. Gopinathan, N. Sathyamurthy, P. K. Chattaraj, R. Ramaswamy, S. Pal, S. K. Ghosh and S. R. Gadre have helped shape this symposium into India's flagship forum for theoretical and computational chemistry. TCS-2025 continues this rich tradition and brings together 648 participants, including 108 plenary and invited speakers, of whom 22 are from abroad, as well as 36 short-talk presenters, 53 session chairs, and 362 posters, with more than 20 poster presenters joining from international universities. A remarkable aspect of this year's symposium is that over 45% of all speakers, chairs, and student presenters are women, reflecting the strong and growing global leadership of women in theoretical and computational chemistry. The scientific program spans electronic structure methods, multiscale simulations, statistical mechanics, reaction dynamics, data-driven and machine-learning approaches, soft and biological matter, and computational materials science, with additional contributions from researchers in industry, highlighting the expanding role of theory and computation in innovation and materials design. This abstract booklet captures the breadth and vibrancy of contemporary research across these domains. We gratefully acknowledge the generous support of our sponsors from industry—HPE-Precision, Micropoint, Lenovo, NVIDIA, AMD, DataDirect, Locuz, Benchmark, Netweb India, Applied Materials, ACS, RSC, Wiley, Springer—and from government funding agencies including ANRF, DBT, BRNS, as well as IoE funding from IIT Bombay, whose contributions have made this symposium possible. We warmly welcome all participants to IIT Bombay and wish everyone an inspiring, engaging, and memorable TCS-2025.



Professors. Gopalan Rajaraman and Rajarshi Chakrabarti
Conveners

Name	Page No.	Abstract Title
Keshavamurthy Srihari	PL1	Vibrational Strong Coupling: Rabi, Rate, and the Riddle
Joan-Emma Shea	PL2	Self-Assembly of the Tau Protein: Liquid-Liquid Phase Separation and Fibrillization
Andreas Dreuw	PL3	Algebraic diagrammatic construction schemes for molecular computations
Raghavan B. Sunoj	PL4	Computational Chemistry and Machine Learning Approaches in Chemical Catalysis
Parbati Biswas	PL5	How do Inhibitors Affect Aggregation of Intrinsically Disordered Proteins?
Balasubramanian Sundaram	PL6	Modelling Molecular Liquids at DFT Level through Machine-Learned Potentials: New Insights
Martin Head-Gordon	PL7	Frontiers in Wavefunction Theory: Regularization, Linear Scaling and Embedding
Graham Worth	PL8	Simulating Photo-Excited Processes using Quantum Dynamics with Grids and Gaussian Wavepackets
Deva Priyakumar U	IL1	Inverse Design Methods for AI Assisted Robotic System for Self-Driving Chemistry Lab
Arnab Bhattacherjee	IL2	Understandingh Protein–DNA Recognition Across Scales
Alexey A. Popov	IL3	Playing with spins inside carbon cages: How theory can be of help
Kalisankar Bhattacharyya	IL4	Atomistic Insights into Electrochemical Heterogenous Catalysis
Susmita De	IL5	Protein-Polymer Structure Reorganization and Higher Order Cooperativity Drives PET Hydrolysis: Peering through a Blackhole
Rukmankesh Mehra	IL6	Computational insights into atypical kinetics, mutation effects and drug-drug interactions in cytochrome P450
Sai Ganesh Ramesh	IL7	Excited State Proton Transfer in 2-(Oxazol-2-yl)-3-hydroxychromone and its Dimers with Water
Mudit Dixit	IL8	From Density Functional Theory to Machine-Learning Potentials: Theoretical Tools for Designing Stable, High-Capacity Battery Materials
Jagannath Mondal	IL9	Integrating Biomolecular simulation with Artificial Intelligence
Jer-Lai Kuo	IL10	Ab Initio Anharmonic Algorithm to understand the quantum resonance revealed by experimental vibrational spectra
Bidisa Das	IL11	Oxyhydroxide Nanostructures in Water:Structure and OER Activity
Anirban Misra	IL12	Design of (4n+2)π cyanide acceptor based 5,7,12,14-tetraazapentacene derivatives as ambipolar organic semiconductors
Kousik Samanta	IL13	Chasing Metastable States: The Multiconfigurational Way
Bhaskar Mondal	IL14	Electronic Structure and Reactivity of Metal-Bound Nitrene Intermediates
Swapan K Pati	IL15	A Multiscale Modeling Approach to Understand Thermal Conductivity and Thermoelectric Properties of Materials

Ram Kinkar Roy	IL16	Investigating the Bimolecular Quenching Rate of Electron Transfer Reactions from Aromatic Amines to Coumarin Dyes: A Conceptual Density Functional Theory-Based Approach
Susmita Roy	IL17	EVOLVE: Integrating Statistical Mechanics and AI for Forecasting Protein Mutation
Prabhat K. Sahu	IL18	Computational Techniques in Drug Design: Emerging Trends & AI Integration
Konstantinos D. Vogiatzis	IL19	From Electronic Structure to Topology: AI-Guided Exploration of Iron-Based Molecular Complexes for Oxidation Reactions
Anik Sen	IL20	In Silico Screening of Natural and Synthetic Compounds as Potential Inhibitors of Tumor-Promoting Ornithine Decarboxylase
Peter Comba	IL21	Modeling spin for applications of metal complexes
Anatoly Kolomeisky	IL22	Dynamic Catalysis as a Novel Strategy For Efficient Chemical Transformations
K. V. Jovan Jose	IL23	New Developments Involving Graph Neural Network-based Algorithms for Structure Prediction and Global Optimization
Pradipta Bandyopadhyay	IL24	Liquid State Integral Equation Theory to Study Biological Processes in complex ionic environments
Dmitrii E. Pradipta	IL25	Static vs dynamic rough energy landscapes: Where is diffusion faster?
Upakarasamy Lourderaj	IL26	Dynamical Origins of Stereoselectivity in the Thermal Deazetization of 2,3-diazabicyclo[2.2.1]hept-2-ene
Saurabh Kumar Singh	IL27	Correlating Electronic Structure, Covalency and Magnetic Anisotropy in f-elements
Pushpita Ghosh	IL28	Spatiotemporal dynamics and emergent orders in chemical and biological systems
Venkatesan Subramanian	IL29	Development of lead Molecules with Antiviral Properties using computational Tools
Bibhu Dash	IL30	HPE And Precision Infomatic
Dimitrios A. Pantazis	IL31	How Photosynthesis Works: Insights from Multiscale Simulations
Kaushik Talukdar	IL32	Relativistic electronic structure calculations for spectroscopic properties of heavy-elemental compounds
Paranjothy Manikandan	IL33	Classical Trajectory Simulations of Gas Phase SN2 Reactions
Nico Van Der Vegt	IL34	The Hidden Choreography of Ions in Acid-Base Chemistry: A Constant pH MD Perspective
Raja Ghosh-1	IL35	Vibronic Quantum Algorithms for Spectroscopy and Dynamics
Muthukumar Kaliappan	IL36	The Interesting Chemistry Talk
Ankan Paul	IL37	Shedding light on the Mechanism of Metal-free, Ultrafast Activation & Functionalisation of C-H bonds exploiting Photo Induced Charge-Transfer in Host-Guest systems

John Mcgrady	IL38	On the interplay between metal-metal and metal-ligand bonding in Zintl clusters: complementary perspectives from DFT and MC-SCF
Sudhakar Yerneni	IL39	AMD
Neetu Goel	IL40	Engineering power conversion efficiency of porphyrin sensitizers for DSSC through metal, ligand and bridge modification: a DFT study
Balamurugan Kanagasabai	IL41	Mechanistic understanding on the potential of graphene-based nanoflakes in inhibiting the Aβ42 aggregation.
Amartya Bose	IL42	Insights into Transport in Aggregates: Path Integral Approaches
Rakesh Singh	IL43	Unraveling Intracellular Protein Phase Separation with Minimal Models
Nayana Vaval	IL44	Non radiative decay processes in weakly bound systems
Azaj Ansari	IL45	Understanding the Reactivity Trend of High Valent Metal-oxo Species towards C-H Activation
Tarak Karmakar	IL46	Machine Learning and Multiscale Modeling Approaches in Molecular Simulations
Manish Modani	IL47	Nvidia
Rajib Biswas	IL48	Vibrational Spectroscopy Modeling to Study Aqueous Systems
Michael Klein	IL49	Remembering Seymour Cray: Architect & Builder of Supercomputers
Upendra Harbola	IL50	Spectroscopy with quantum light
Michal Repisky	IL51	Relativistic Real-Time DFT: Probing Light-Induced Ultrafast Phenomena
G. Narahari Sastry	IL52	Criterion to Characterize Non-Covalent Interactions and Their Cooparativity
Divya Nayar	IL53	Computational design of stimuli-responsive biopolymer-grafted nanoparticles for therapeutics
Sudip Chakraborty (Cup Punjab)	IL54	Mechanistic Aspects of SWCNT Dispersion in RTILs
Susanta Mahapatra	IL55	Quantum Dynamics of Chemical Systems of Astrophysical Interest
Soumen Ghosh	IL56	Why Variational Density Functional Theory Is More Accurate Than Time-Dependent Density Functional Theory for Certain “Difficult” Excited States?
Anirban Mondal	IL57	Dark Light, Smart Design: Cracking the Code of NIR-TADF with ML-Guided Inverse Design
Martin Srnec	IL58	Thermodynamic principles for regulating of H-atom abstraction reactivity
Priyadarshi Satpati-1	IL59	When Molecules Meet: MD Simulations Illuminate Biomolecular Recognition
Prabha Vadivelu	IL60	Tuning the reactivity of MnIII-O2/OOH species in catalytic oxidation reactions: A DFT study
Federico Totti	IL61	Three irons on a sombrero: vibronic acrobatics and magnetic marvels on a Mexican hat

Sudip Chakraborty (Hri Allahabad)	IL62	Computational Advancement towards Efficient Energy Materials:Connecting a Few Dots
Deepa Janardanan	IL63	Impact of Microplastic Structure and Aging on Cefixime Adsorption Dynamics
Andrew M. Rappe	IL64	Coupled Electronic, Structural, and Dynamical Optoelectronic Responses in Nanomaterials
Avisek Das	IL65	Role of protein-protein interactions in molecular mechanism of biological copper trafficking
Prakash Muthuramalingam	IL66	Functionalized MOFs for Selective CO2 Capture and Conversion
Pinku Nath	IL67	CHEMONTO: Leveraging Chemical Knowledge for Smarter Reaction Network Exploration
Md. Mehboob Alam	IL68	Our recent attempts in computational designing of photosensitizer for photodynamic therapy application
Govardhan Reddy	IL69	Transition Metal Ion Sensing by Riboswitches
Anoop Ayyappan	IL70	Uncovering Structure in Chemical Space: Automated and Data-Driven Approaches
Raghunath O. Ramabhadran	IL71	How to Generate Unique Machine Readable Representations of Conformers, Tautomers, Transition States, Excited States, Molecular Clusters, Non-Equilibrium Geometries and Potential Energy Surfaces?
Debasish Mondal	IL72	Brownian Information Engines: The Essentials for Best Performance
Charulatha Venkatara	IL73	Reduced density matrix approaches to describe photoinduced proton-coupled electron transfer
Somrita Ray	IL74	Stochastic Resetting Prevails Over Sharp Restart for Broad Target Distributions
Pallavi Debnath	IL75	Analytical solutions in model polymer systems
Niladri Patra	IL76	pH-Driven OprM Gating and Allosteric Control in MexAB-OprM/AcrB Efflux Pumps
Amit Kumar Paul	IL77	Capturing Vibrational Excitation Patterns of Molecular Systems using Machine Learning Tools
Biman Jana	IL78	Optimizing collective variable and enhancing protein folding transitions with explainable machine learning model: Role of hydration
Prashant Manohar	IL79	Equation of motion coupled cluster with singles, doubles and full triples: Some pilot applications
Puneet Gupta	IL80	Computational Insights into Boron-Catalyzed Small-Molecule Activation: From Methane Oxidation to CO2 Utilization
Hemant K. Kashyap	IL81	Lipid Vesicle Behavior in Ethanolic Environment: Swelling, Rupturing, Aggregation, and Fusion
Srinivasu Kancharlapalli	IL82	Computational Studies to Explore Metal Organic Framework Materials for CO2 Capture from Flue Gas Mixture
Shivnath Mazumder	IL50	AI-Driven Discovery of Asymmetric Pauson-Khand Reactions: A New Toolbox in a Synthetic Chemist's Treasure

Pralok Kumar Samanta	IL84	Modelling of Excited State Properties in Narrow-Band Organic Emitters
Raghunathan Ramakrishnan	IL85	Computational prediction of new molecular candidates for delayed fluoroscence from inverted singlet and triplet states
Vamsee Voora	IL86	Resolving Density-Driven Errors in Kohn—Sham and Post Kohn—Sham Methods: From Molecules to Materials
Nisanth N. Nair	IL42	Buckets Instead of Umbrellas for Enhanced Sampling and Free Energy Calculations
Jayashree Nagesh	IL88	Using Deep Learning models to predict mixed quantum-classical trajectories
Shubhra Ghosh Dastidar	IL89	Insights into the Molecular Mechanisms in Biology using Modeling and MD Simulations
Ravi Venkatramani	IL90	Integrating Multiple Electronic Pathways in Single Molecule Breadboard Junctions
Padmesh Anjukandi	IL91	Towards the binding of S-Peptide to S-Protein in the S-Peptide S-Protein Complex (RNase S)
Alessandro Soncini	IL7	Preparation and coherent manipulation of toroidal moments in molecules
Suman Chakrabarty	IL93	Enhanced Sampling and Estimation of Rare Event Kinetics in Molecular Simulation: Some Ideas and Benchmarks
Sangita Sen	IL94	Modelling Excited States : Insights from Selected Examples
Yesodharan Sajeev	IL95	Bond Breaking, Bond Making, Activating, Catalyzing: Low-Energy Free Electrons as Tunable Reagents
Sanjay Kumar	IL96	Quantum Dynamics Studies of Charge-Transfer Processes in Ion-Molecule Collisions at High (keV) Collision Energies relevant to Cometary Environments
Sandeep Kumar	IL97	Etching Silicon Oxide – Catalysis and Selectvity
Nicholas T Bronn	IL98	Quantum Computing for Computational Chemistry
Rajeev Ramanan	IL99	Frontiers in Wavefunction Theory: Regularization, Linear Scaling and Embedding
Vidya Avasare	IL100	Chirality Without Chiral Sources: Computational Insights
Gopi Chandran	IL101	AMAT
ParthaPratimPal	IL102	Wiley
Imon Mandal	SOP1	Unravelling Atmospheric Reaction Mechanisms at Seawater: Insights from Ab-Initio Molecular Dynamics Study
Sruthi Sudhakar	SOP2	Transient Occupancy and Pore Dynamics: IP6 behavior in HIV-1 T=4 Capsids
Ankita Narwal	SOP3	Interfacial stability of Electrolytes at pure and oxidized Mg surfaces- Insights from Ab Initio Molecular Dynamics
Nandu P S	SOP4	Fundamental Underpinnings of Ion-π Interactions: Essence and Nature
Dyuti Chatterjee	SOP5	Machine Learning Boosted Quantum-Profiling of Blood Antigens
Prashant Kumar	SOP6	Unveiling the Mechanisms of Excited-State Formation in Radical-Based Organic Light-Emitting Diodes

Sisodiya Dilawar Singh	SOP7	A Computational Study on cis–trans Photo and Thermal isomerizations of Azobis(benzo-15-crown-5) and its Metal Ion Complexes
Aanchal Grover	SOP8	Second-Order Saddle Points and Concerted Reaction Mechanism: Insights from Entangled Trajectory Molecular Dynamics
Vaibhav Bhatt	SOP9	Different Water Architecture Diversifies the Catalytic Activity in Two Deceptively Similar Cytochrome P450 Isozymes
Atreyee Majumdar	SOP10	Unlocking Inverted Singlet–Triplet Gap in Alternant Hydrocarbons with Heteroatoms
Tanwi Debnath	SOP11	Cellular uptake of microgels by membrane wrapping
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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Vibrational Strong Coupling: Rabi, Rate, and the Riddle

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Can a ``dark" optical cavity influence chemical reaction dynamics? If one were to take a cue from decades of research in cavity quantum electrodynamics and quantum optics then the answer to the question should be a resounding yes! Indeed, the prospect is exciting: using quantum vacuum fluctuations in a cavity to create Rabi-split light-matter hybrid states (polaritons) and, in doing so, modulate chemistry at will. However, some experiments have observed substantial rate modification, while others have shown almost no effect. Perhaps, this is due to the fact that molecules are neither simple two-level systems nor are their vibrations purely harmonic. At the same time, despite a focused effort by theoreticians, a predictive theory of vibrational strong coupling-mediated chemistry still eludes us.

This talk will summarize our theoretical insights gained from studying simple models, *based on the hypothesis that further progress requires an understanding of how strong coupling to the cavity influences intramolecular vibrational energy flow pathways in molecules*. Apart from revealing the significance of coherent cavity-molecule energy transfer under resonant conditions, our models also exhibit surprisingly good classical-quantum correspondence. The talk concludes by highlighting the limitations of these model systems and discussing the outstanding challenges that remain in the field of vibrational strong coupling.

[*] Work done by Mr. Subhadip Mondal and Mr. Atul Kumar.

Self-Assembly of the Tau Protein: Liquid-Liquid Phase Separation and Fibrillization

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Intrinsically disordered proteins (IDPs) belong to a class of proteins that do not fold to a well-defined, three-dimensional structure, but rather co-exist between interconverting, partially structured conformations. In the crowded cellular milieu, IDPs can form liquid droplets through liquid-liquid phase separation or self-assemble into beta-sheet-enriched amyloid fibrils, processes linked to normal physiological functions and various pathologies. In this talk, I will present a new computational framework that scores amyloid and LLPS propensities from protein language model (pLM) embeddings, thereby enabling rapid proteome-wide annotation of peptides and residues. We apply these frameworks to the Tau protein, an intrinsically disordered protein that plays an important role in stabilizing microtubules, and identify segments of Tau that have a propensity to phase separate or form fibrils. Using a multiscale approach combining atomistic, coarse-grained, and field-theoretic simulations, we further characterize the mechanisms of fibrillization and phase separation of these fragments and shed light on the sequence characteristics linked with these two modes of assembly.

Algebraic diagrammatic construction schemes for molecular computations

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Algebraic diagrammatic construction (ADC) schemes represent a family of ab initio methods for the calculation of excited electronic states, electron-detached and -attached states. All ADC methods have been demonstrated to possess great potential for molecular applications, e.g., for the calculation of absorption or photoelectron spectra or electron attachment processes. ADC originates from Green's function or propagator theory, however, our most recent ADC developments heavily rely on the intermediate state representation (ISR), which comprise new ADC methods and computational schemes for high-order properties. The different approaches for the calculation of excitation energies (EE-ADC), ionization potentials (IP-ADC) and electron affinities (EA-ADC) are intimately related, and provide a coherent description of these quantities at equivalent levels of theory and with comparable errors. Recent developments of ADC schemes and the closely related unitary coupled cluster (UCC) methods will be shown and their relation discussed.

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Computational Chemistry and Machine Learning Approaches in Chemical Catalysis

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Abstract

Computational science is an enabling technology capable of accelerating growth and for offering detailed insights into problems in a given domain of research. For instance, computational quantum chemistry has been increasingly employed toward rationalizing the stereochemical outcome of catalytic reactions.[1] In our laboratory, density functional theory computations are employed to gain insights into stereoselective reactions of immediate practical significance.[2] The key objective of our research is to decipher the factors responsible for stereoselectivity and to harness such knowledge toward *in silico* design of novel asymmetric catalysts.[3]

In general, the presentation would encompass a few contemporary themes in the domain of asymmetric multi-catalytic reactions. The process of chirality transfer from the catalysts to the developing stereogenic center(s) in the product could be understood with the help of our computed transition state for the enantio-/diastereo-controlling step in the catalytic cycle. In keeping with the latest developments in multidisciplinary research, we have been trying to tap the potential of machine intelligence for chemical catalysis.[4] An overview of how machine learning models, built on intuitively chosen molecular descriptors or by using chemical language model, could be exploited in asymmetric catalysis as a way to develop high-throughput methods will also be presented.[5] In addition, a critical assessment of whether computational chemistry and/or ML driven predictions can actually work under the wetlab conditions would be demonstrated.[6] The contents are designed to cater to a broad and diverse group of audience; hence, the chemical insights would be emphasized, rather than a labyrinth of technical details.

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How do Inhibitors Affect Aggregation of Intrinsically Disordered Proteins?

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Protein aggregation in a cellular environment has been associated with numerous neurodegenerative pathologies like Alzheimer's, Huntington's, and Parkinson's diseases. Intrinsically disordered proteins (IDP) are more prone to aggregation as compared to globular proteins. These proteins are involved in a wide range of cellular functions and typically exist as an interconvertible ensemble of fluctuating conformations, which are difficult to characterize experimentally under standard physiological conditions. Alzheimer's disease is specifically linked to the misfolding of amyloid-β (Aβ) and tau proteins to form highly organized protein aggregates called amyloid-fibrils. Recent experimental studies confirm that soluble oligomers rather than insoluble fibrils predominantly contribute to synaptic dysfunction and neuronal death. Inhibiting aggregation of Aβ and tau proteins may be an effective therapeutic strategy to prevent or delay the onset of this disease. The aggregation of amyloid-β (Aβ-42) and its mutants are investigated by a combined approach of all-atom explicit water MD simulations and 3D-RISM theory. The effect of inhibitor on the aggregation propensity of full length Aβ-42 and PHF6 derived from the tau protein is also investigated along similar lines. Results highlight key contributions of different interactions present in the amyloid oligomers.

Modelling Molecular Liquids at DFT Level through Machine-Learned Potentials: New Insights

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The advent of Car-Parrinello molecular dynamics (CPMD) simulation method in 1985 demonstrated the possibility of time evolving nuclear coordinates (albeit classically), not on a fixed potential energy surface as in empirical force field based MD, but one where the potential energy surface (PES) is determined via quantum density functional theory (DFT) at each time step. Despite this significant breakthrough, CPMD or its variant, Born-Oppenheimer MD (BOMD), was utilized more as an exotic surgical tool, due primarily to its large computational requirements. The development of machine learning methods to represent the interatomic environment and atom energies and forces has allowed MD simulations over instantaneous DFT-defined PESes to be performed at ease, on GPU-based computing platforms. Over the last five years, machine-learned interatomic potentials (MLIPs) have matured significantly, and several foundational models are now available that work for multiple chemical systems with little or no finetuning.

In this talk, I shall illustrate the development and use of MLIPs to model aqueous salt solutions[1,2], molecular fluids[3], and inorganic glasses[4]. These examples demonstrate the accuracy of de novo MLIPs toward the quantitative prediction of molecular diffusion, conformer populations, and intermediate range structural order.

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Frontiers in Wavefunction Theory: Regularization, Linear Scaling and Embedding

Martin Head-Gordon,

Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Simulating Photo-Excited Processes using Quantum Dynamics with Grids and Gaussian Wavepackets

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Simulating the time-evolution of molecular systems after photo-excitation is complicated by the need to include a manifold of excited electronic states. These states are coupled by so-called non-adiabatic coupling due to the interaction of the electronic and nuclear motion which makes the system highly quantum mechanical. As a result it is necessary to solve the time-dependent Schroedinger Equation (TDSE) for reliable results. To solve the TDSE, however, is a hard computational problem due to the exponential scaling of required resources with system size. The multi-configuration time-dependent Hartree (MCTDH) method provides a suitable algorithm that efficiently contracts the wavefunction to make it manageable for many degrees of freedom [1]. Such simulations can provide a full description of the evolving system, and it is possible to include the excitation by light pulses to obtain a spectroscopic signal that can be directly compared to experiments, such as REMPI spectra [2]. These simulations, however, are constrained by the need for an analytic Hamiltonian, which is usually unable to describe long-range motions. For this, methods such as the direct dynamics variational multi-configuration Gaussian (DD-vMCG) method [3] are required that calculate the potential surfaces on-the-fly and so allow a flexible description of the long-time molecular response [4].

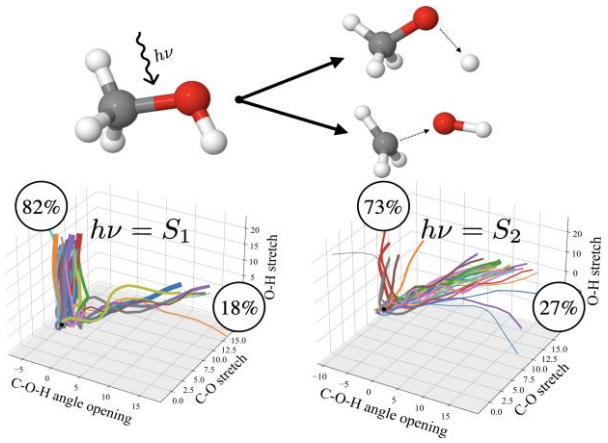


Figure 1 Methanol photodissociation

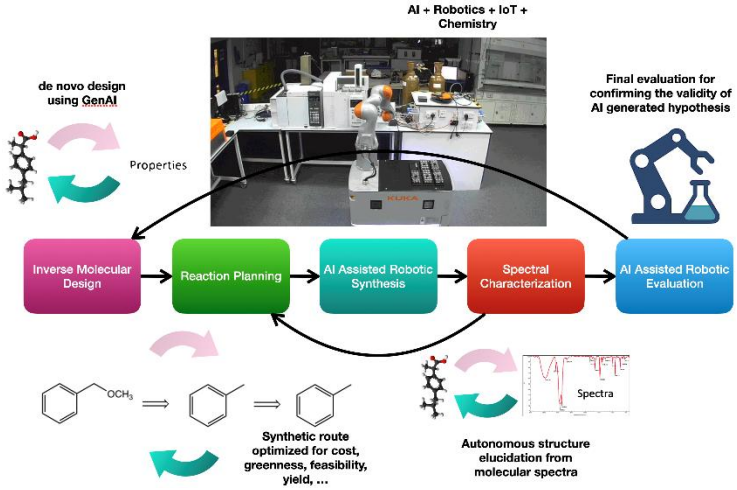
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Inverse Design Methods for AI Assisted Robotic System for Self-Driving Chemistry Lab

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Autonomous or Self-driving labs integrate artificial intelligence (AI)/machine learning (ML) models, robotics and high-throughput experiments to enable molecular design, experimental synthesis & testing and further optimization of the design for identifying molecules/materials for specific purposes with minimal human intervention. It is a closed loop system that consists of AI models (forward and inverse) that propose hypothesis, perform AI assisted robotic synthesis and characterization, and improve the AI models based on the new experimental data thereby advances chemical experiments towards improved safety, reproducibility, efficiency and reliability. In this talk, we will present an inverse desgin approach that takes molecular properties as input and gives potential molecules with these property values as output. A model developed based on generative pre-trained transformer (MolGPT) to understand drug-like molecules will be discussed. MolGPT is capable of generating chemically valid and novel molecules and can be conditioned to satisfy the requirements of the user. Improvement to this model, MolGPT2.0, is done using direct preference optimization (DPO), wherein the conditioning could be achieved complex molecular properties such as shape and electronic compatibility of the generated molecule with respect to given protein structures. Discussion on how inverse design tasks such as this are crucial in achieving self-driving chemistry laboratories.



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Understandingh Protein–DNA Recognition Across Scales

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Abstract: How do proteins know where to bind on the DNA? This simple question hides an extraordinary journey — one that spans from the random motion of molecules to the organized architecture of the genome. Proteins search for their specific DNA sites, guided not only by sequence but also by the DNA's flexible shape. In eukaryotic cells, this search becomes even more complex as DNA is wrapped around nucleosomes and folded into higher-order chromatin structures. These dynamic layers of organization influence which genes are accessible and when they are expressed.

In this talk, I will trace this journey — from molecular diffusion and DNA deformation to nucleosome wrapping and the 3D folding of the genome. Using a combination of physical modeling, simulations, and experimental data, we uncover how the genome's structure encodes "decisions" that underlie gene regulation, development, and disease.

Playing with spins inside carbon cages: How theory can be of help

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Encapsulation of magnetic species within robust molecular containers is a natural route towards stable and processable single molecule magnets (SMMs). Air-stability, thermal stability, ability to form thin molecular layers on different substrates are among the critical issues to be addressed. Chemical and thermal stability of fullerenes makes them perfectly suitable for this goal. When fullerenes encapsulate rare-earth metal atoms, the latter can form single-electron metal-metal bond, resulting in peculiar magnetic properties, such as giant exchange coupling or very broad magnetic hysteresis.[1] Metallofullerenes can be sublimed and form monolayers on differnet substrates, and yet retain their magnetic properties.[2,3] In this contribution we will overview the studies of magnetic metallofullerenes synthesized in IFW Dresden and demonstrate how computational studies go hand and hand with experiemtnal explortation of these fascinating materials.

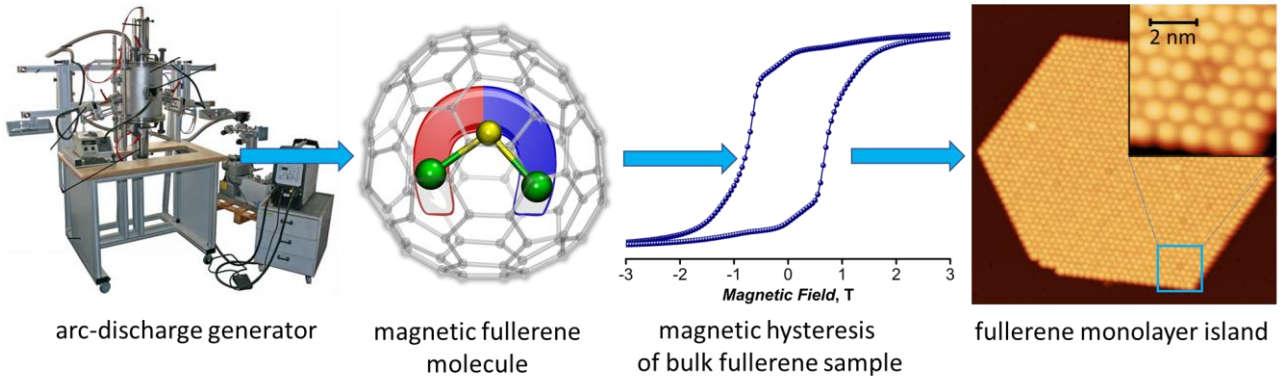


Figure 1 Life cycle of magnetic endohedral fullerene: from synthesis to surface deposition. At each step, theoretical MD, DFT, or CASSCF computations augment experiment.

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Atomistic Insights into Electrochemical Heterogenous Catalysis

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Abstract: In this invited talk, I will discuss the critical roles of constant potential and spin states in layered hydroxide-based electrocatalysis for the oxygen evolution reaction (OER). We present a comprehensive computational study on single-atom iron-doped graphene catalysts under constant potential conditions. A new simulation protocol is developed, based on grand canonical quantum mechanics and on-the-fly potential control, to accurately capture electron transfer dynamics throughout the reaction pathway. This methodology enables the prediction of structural evolution as a function of applied potential and pH.[1] Our results demonstrate that axial ligand coordination on single-atom catalysts significantly modulates the spin state, directly impacting catalytic activity. Spin-polarized DFT and ab initio molecular dynamics (AIMD) calculations reveal that single atom Fe exhibits the lowest overpotential, governed by the *OOH formation step as the potential-determining step (PDS), while larger clusters are limited by *O formation. Crystal orbital Hamilton population analysis and adsorption energy scaling relationships provide mechanistic insights and guide strategies for optimizing multi-Fe site catalysts through *OH binding energy modulation.[2]

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Protein-Polymer Structure Reorganization and Higher Order Cooperativity Drives PET Hydrolysis: Peering through a Blackhole

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PET hydrolysis is a complex, dual-phase enzymatic challenge where substrate recognition and reactant complex formation are distinct from the bond-breaking step.[1,2] Unlike small-molecule catalysis, PET hydrolysis involves multiple enzyme surface adsorption sites with both direct and inverse correlations between amino acids and binding energies. Conformational rearrangements at protein-polymer interfaces and higher-order cooperativity among residues strongly influence the relative stabilities of reactants, intermediates, and products.[3,4] This leads to a “black hole” of uncertainty. Though product formation is evident, the detailed molecular orchestration of catalysis remains elusive. Using PETase as a model, the study highlights how structural dynamics and catalytic efficiency emerge from the intricate protein-polymer interaction landscape, underscoring the need for integrative multi-scale approaches to resolve this complex system.

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Theoretical Chemistry Symposium
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Computational insights into atypical kinetics, mutation effects and drug-drug interactions in cytochrome P450

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Cytochrome P450 (CYP450) constitutes an important superfamily of heme-containing enzymes that mediate the metabolism of drugs and xenobiotics. 57 CYP450 enzymes are known in humans. These enzymes do not always follow Michaelis-Menten kinetics and multiple ligands bind simultaneously to the active site. CYP450 enzymes have a broad substrate-binding site and a conserved heme-binding domain. More than 200 pathogenic mutations have been identified across different CYP450 isoforms. Given their central role in xenobiotic clearance, CYP450s are also important contributers of drug-drug interactions. To elucidate the molecular basis of their atypical kinetics, we investigated CYP3A4 (Figure 1) using 21 μs of molecular dynamics simulations, focusing on ligand binding at both the active and allosteric sites.[1] To explore the reason for the pathogenicity of mutations, we computed folding stability landscapes across 26 CYP450 isoforms, covering 25,94,151 mutation effects, with eleven sequence- and structure-based methods.[2] This analysis consistently revealed the stability trend: non-pathogenic > all-possible > pathogenic mutations. In addition, we developed a deep learning framework, UniGEN-DDI, to predict drug-drug interactions by integrating GraphSAGE and Node2Vec on DrugBank v5.0.1.[3] Its predictive power was validated against a newly curated dataset from DrugBank v6.0. Overall, this study provides a comprehensive view of cytochrome P450 enzymes, spanning mechanistic insights into their non-classical kinetics, systematic evaluation of mutational pathogenicity, and machine learning-based prediction of drug interactions.

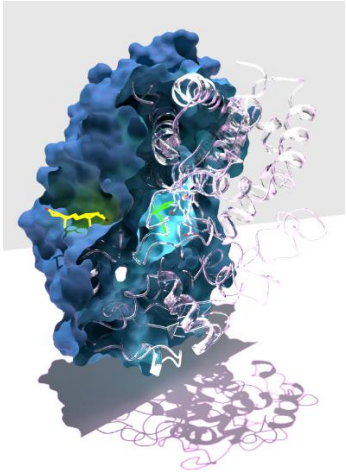


Figure 1 CPY3A4 showing ligand binding to active (green stick) and allosteric sites (yellow stick).

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Excited State Proton Transfer in 2-(Oxazol-2-yl)-3-hydroxychromone and its Dimers with Water

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The molecule of interest, 2-(oxazol-2-yl)-3-hydroxychromone or OHC, is a derivative of the well-studied 3-hydroxychromone. OHC has three low-energy conformers in the gas phase arising from the OH torsion and rotation about the CC bond bridging the chromone and oxazole rings. Two of them, OHC-A and B, have OH···O H-bonding within the chromone ring, while OHC-C has OH···N H-bonding between the chromone and oxazole rings.

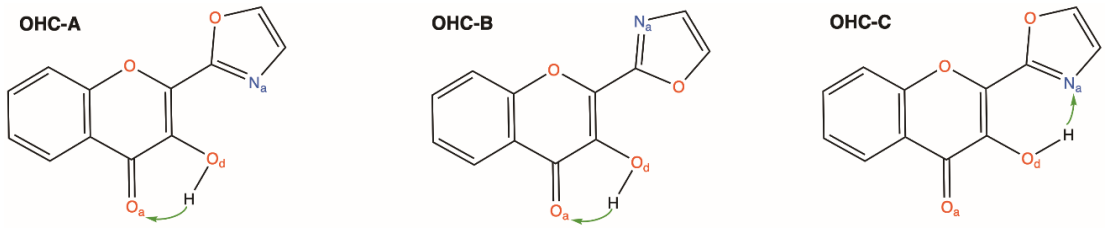


Figure 1 Conformers of OHC

We have investigated the energy landscape and dynamics of the proton transfer (PT) of these conformers in the gas phase. OHC-B and C are found to be similar in energy while OHC-A is slightly higher. At the TDA-B3LYP level, the potential profiles show lower barriers to PT for OHC-A and B than OHC-C on the lowest bright state (S_1 for A and B, and S_2 for C). Fewest-switches surface hopping simulations, initated on both S_1 and S_2 states for these conformers, shows different propensities for intra-ring (OHC-A and B) and inter-ring (OHC-C) proton transfer. Through the potential profiles and simulations, we have tried to understand the PT dynamics as well as the fluorescence behaviour of the OHC confomers.

Extending this study, we have investigated water-mediated PT in each of the three conformers. Based on their relative energies, OHC-B•H_2O and OHC-A•H_2O dominate the population, in that order, while OHC-C•H_2O is expected to have negligible population. Following a computational study, we have analysed the dynamics of the PT process initiated on the first bright state in each case. For OHC-A•H_2O and OHC-B•H_2O, both double PT (donor-water and water-acceptor) and single PT events are found. The double PT events also show distinct features depending on whether they are of the donor-first or acceptor-first types. In contrast, OHC-C•H_2O shows mostly DPT events. The details of the dynamics and the contrast of the monomer and dimer PT propensities will be discussed.

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From Density Functional Theory to Machine-Learning Potentials: Theoretical Tools for Designing Stable, High-Capacity Battery Materials

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In this talk, I will present our recent efforts to stabilize and understand layered metal oxide cathodes for Li-and Na-ion batteries, with a particular focus on anionic redox and the inherent trade-offs between structural stability and capacity. Using Density functional theory calculations, we offer key insights into electrochemical and phase stability under cycling conditions. I will also highlight the use of Machine Learning Interatomic Potentials (MLIPs) as a powerful tool for accelerating materials discovery. We critically evaluate their application in single-atom catalysis and Li-S batteries, particularly in modeling polysulfide binding, while also discussing our newly developed approach to accurately identify the adsorbate sites and their configurations. Additionally, I will also discuss the design of a series of layered transition metal oxide cathodes, where anionic redox can be stabilized to achieve high capacities reversibly. Through electronic structure engineering, our goal is to develop materials that not only exhibit reversible anionic redox activity but are also stable in air and moisture, including novel multi-component compositions. Our findings provide fundamental understanding and provide valuable guidance for experimental efforts aimed at enhancing existing materials and designing next-generation cathode materials.

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Integrating Biomolecular simulation with Artificial Intelligence

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Generative Transformer models, originally designed for natural language processing, are emerging as powerful tools in biomolecular simulations and sequence design. In this seminar, we present two distinct yet complementary applications of the Generative Pre-trained Transformer (GPT) framework to address long-standing challenges in molecular biophysics. First, we demonstrate that GPT can effectively learn the time evolution of biomolecular systems by treating molecular dynamics (MD) trajectories as discrete sequences akin to language corpora. This enables accurate and efficient prediction of kinetic state-to-state transitions, even for out-of-equilibrium systems, with the model's self-attention mechanism playing a central role in capturing long-range correlations in conformational space. Second, we explore the role of GPT in decoding the molecular grammar of proteins undergoing liquid-liquid phase separation (LLPS). By training on curated datasets of LLPS-prone and resistant proteins, GPT models learn distinguishing sequence features and generate de novo peptides with phase-separating potential. Experimental validation confirms the ability of these synthetic peptides to undergo LLPS in vitro. Together, these studies highlight the potential of transformer-based generative models to advance biomolecular simulation and rational design of phase-separating proteins, offering a unified framework to address structural dynamics and functional sequence generation.

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Ab Initio Anharmonic Algorithm to understand the quantum resonance revealed by experimental vibrational spectra

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In the past two decades, many experimental studies reveal complex vibrational features, between 2800 – 3400 cm^{-1}, of $H_2O\cdots X^-$[1-4], where X = I, Br, Cl, CN, NC, mNP and F. In this talk, we will present our recent theoretical analysis on whether these peculiar vibrational features are results of quantum resonance originates from anharmonic coupling with the low-frequency modes of vibrational motion of H_2O in these complexes.

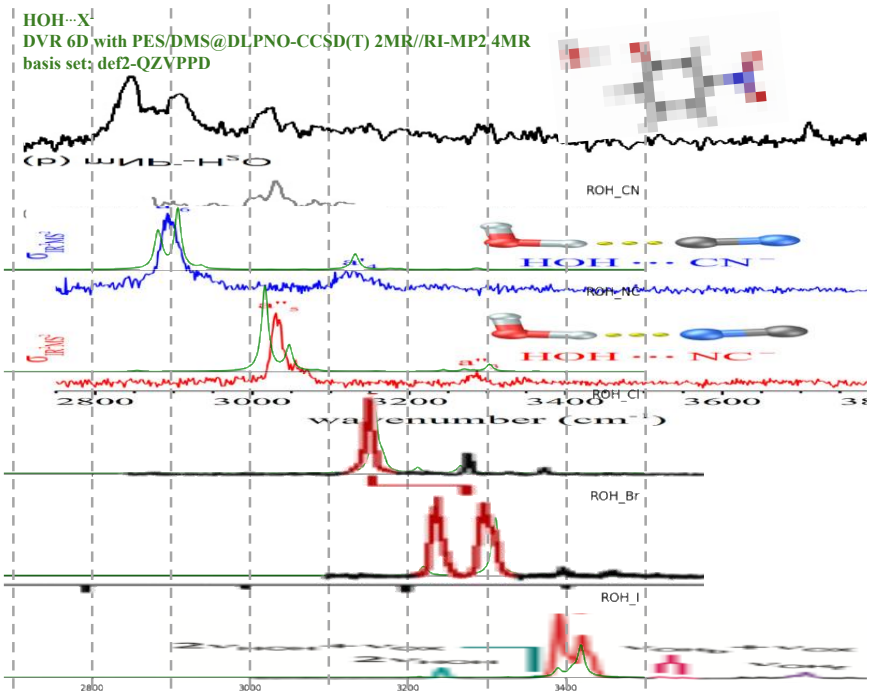


Figure 1 Experimental IRPD spectra of **$H_2O\cdots X^-$** and comparison with simulated absorption spectra (in green) using PES at DLPNO-CCSD(T)/def2-QZVPPD with six degrees of freedom.

References:

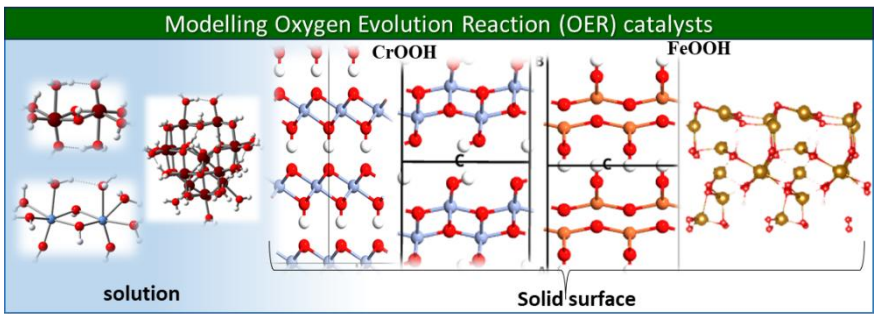
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Theoretical Chemistry Symposium
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Oxyhydroxide Nanostructures in Water:Structure and OER Activity

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Nanostructured metal oxyhydroxide minerals like that of FeOOH/CrOOH are abundant in the environment and are responsible for geochemical cycling of ions. We examined Fe and Cr oxyhydroxides for catalytic applications, especifically for Oxygen Evolution Reaction (OER) as earth-abundant alternatives to conventional ones, which are rare and expensive. The growth of oxyhydroxide minerals involve nucleation of multinuclear oxyhydroxide clusters in aquatic environments during early-stage polymerisation.[1,2] We first explored Fe oxyhydroxide nanoclusters which forms *in-situ* in water, for OER activity, studied the step-wise reactions and calculated the reaction free energies considering acidic, neutral and alkaline environments. We systematically compared the catalytic performances of pure and 3d-transition metal doped Fe oxyhydroxide clusters. We then modelled solid Ferrihydrite surfaces for OER activity as it is the most reactive Fe oxyhydroxide. Our results for Fe oxyhydroxide clusters and surfaces show modest OER activity for Ferrihydrite, but Lepidocrorite is significantly more promising. We then examined various Cr oxyhydroxide polymorphs for OER activity and investigated layered γ-CrOOH surfaces for pristine and defected forms. OER activity of γ-CrOOH was found to be excellent for realistic implementation. The overall understanding of abundantly available metal oxyhydroxide minerals spanning different length-scales helps in their strurural tailorability and most importantly their strategic application as effective catalysts.



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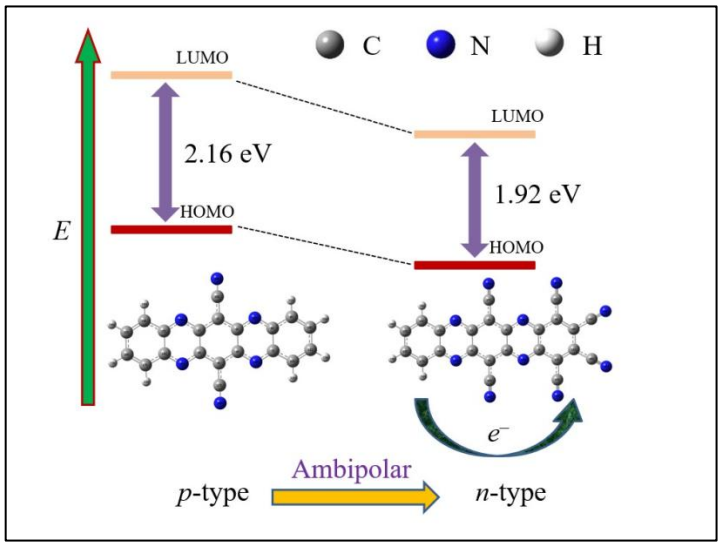
Design of (4n+2)π cyanide acceptor based 5,7,12,14-tetraazapentacene derivatives as ambipolar organic semiconductors

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Abstract

Ambipolar molecules are of significant importance in the field of organic electronics and semiconductor devices primarily due to their dual charge carrier transport nature, which results into simplification of device design, enhanced device performance, tuning of electrical properties and versatility in application. In this study, density functional theory (DFT) based calculations are performed to examine the effects of sequential cyanation (–CN) on the adiabatic ionization potential (IP), adiabatic electron affinity (EA), reorganization energies (λ_h and λ_e) and charge transfer rate ($K^{\neq}$) along with charge (hole and electron) injection possibility for a series of derivatives based on already synthesized 5,7,12,14-tetraazapentacene (N4PENT) as the core moiety. The results illustrate that introducing two or more cyanide (–CN) groups onto the N4PENT core is sufficient to induce stable ambipolar charge transport properties, trending toward n type semiconducting character. Apart from, analysis of the density of states (DOS) offers a clear understanding of how sequential cyanation affects the distribution of electron density. Overall, this study underscores a rational foundation for designing stable ambipolar organic semiconductors (OSCs), which could significantly advance organic electronics, leading to more efficient and adaptable electronic devices applicable in flexible electronics, wearable technology, and low-cost displays.[1]



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Chasing Metastable States: The Multiconfigurational Way

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Negative-ion resonances (NIRs) are transient electronic states that play a pivotal role in diverse physical, chemical, and biological processes—from atmospheric and interstellar chemistry to radiation-induced DNA damage. Despite their ubiquity, the theoretical characterization of NIRs remains a formidable challenge because they exist in the continuum spectrum of the Hamiltonian and require a simultaneous treatment of electron correlation and scattering phenomena.

This talk presents a systematic overview of recent theoretical advances in the study of NIRs, with particular emphasis on the development of **multiconfigurational propagator approaches** augmented by a **complex absorbing potential (CAP)**. The CAP introduces an absorbing boundary condition that effectively transforms the continuum problem into a tractable bound-state one, allowing the use of well-established quantum chemical methods. By integrating CAP within a multiconfigurational self-consistent field (MCSCF) framework, the resulting **CAP-MCSCF propagator theory** provides a balanced description of both static and dynamic electron correlation in metastable systems.

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Theoretical Chemistry Symposium
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Electronic Structure and Reactivity of Metal-Bound Nitrene Intermediates

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Abstract

Metal-bound nitrenes are key intermediates in a variety of biocatalytic and synthetic nitrene-transfer reactions. One of the most intriguing aspects of metal-nitrenes is the complex bonding between open-shell transition metals and redox-active nitrenes, which significantly influences their nitrene-transfer mechanism and reactivity. However, determining the “true” electronic nature of the metal-nitrene bond–and thereby understanding the electronic origins of their reactivity–poses a significant challenge due to their high reactivity.

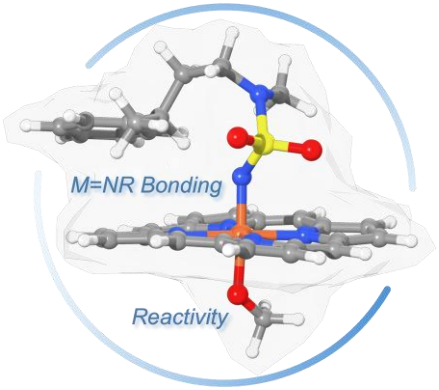


Figure 1 A representative metal-nitrene complex

We utilize advanced quantum chemical techniques, such as density functional theory (DFT), ab initio multi-configurational CASSCF, and CASSCF/NEVPT2 methods, to precisely characterize the metal-nitrene bonding and its impact on reactivity. The first part of this talk highlights the fundamental differences in bonding and reactivity between Co- and Fe-porphyrin-nitrenoid species. The second part demonstrates how the subtle Fe-nitrene bonding interactions are influenced by the ligand environment, leading to unexpected nitrene-transfer reactivity. Finally, using a Co-catalyzed C–H amination reaction as an example, the discussion will emphasize how the metal–nitrene bond governs the reaction mechanism. Overall, our findings underscore the importance of a deep understanding of electronic structure-reactivity correlations in catalytic nitrene-transfer reactions. This knowledge not only unravels the complex electronic factors driving reactivity but also paves the way for the design of more efficient catalysts for targeted organic transformations.

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A Multiscale Modeling Approach to Understand Thermal Conductivity and Thermoelectric Properties of Materials

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The Wigner-Boltzmann transport equations (WBTE) for charge carriers and phonons have been developed in-house along with first principles calculations to model and understand the transport processes in various materials. Using the WBTE equations, we have computed the thermoelectric efficiency in n-type S and Te doped Ag_2Se systems [1] and in 9 Bi based half-Heusler compounds XYBi (X: Ti, Zr, Hf; Y: Co, Rh, Ir) [2]. We also have modelled TlAgSe for finding its thermal conductivity, which was synthesized and investigated experimentally [3]. I shall also discuss our theoretical attempt in finding lower thermal conductivity in $TlIn_{0.5}Ga_{0.5}Te_2$, which was derived from two synthesized and studied systems, $TlInTe_2$ and $TlGaTe_2$ [4].

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Investigating the Bimolecular Quenching Rate of Electron Transfer Reactions from Aromatic Amines to Coumarin Dyes: A Conceptual Density Functional Theory-Based Approach

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Abstract:

An alternative and cost-effective computational approach is used to qualitatively predict the trend of quenching rate of a series of bimolecular electron transfer (ET) reactions. We have correlated the qualitative comparison of the trend of quenching rate constant with the sum of stabilization energy and reorganization energy in bimolecular electron transfer reactions, in the spirit of classical Marcus theory.[1] The electron transfer reactions from eight aromatic amines (in their ground state) to a series of six derivatives of coumarin dyes [in their singlet excited states (S_1)] are selected as representative quenching processes.[2,3] The acetonitrile solvent is used as the reaction medium. The conceptual density functional theory (CDFT) based comprehensive decomposition analysis of stabilization energy (CDASE)[4] scheme is used to compute the values of reaction-free energy. The observed trend of the CDASE scheme-based stabilization energy indicated that it can be used qualitatively as a substitute for experimentally obtained reaction-free energy. The reorganization energy values are calculated using a conventional method (i.e., Marcus Model) already prescribed in the literature.[5] As these reactions proceed under diffusion-controlled conditions, only the solvent reorganization energy plays a predominant role, while the intramolecular reorganization energy is neglected (as suggested by corresponding experimental studies available in the literature).[2,3] It is observed that as the absolute values of the CDFT-based stabilization energy become closer to the corresponding reorganization energy, the experimental bimolecular quenching rate constant values for the chosen weakly coupled donor-acceptor systems increase. These findings are consistent with Marcus theory of electron transfer reaction. Thus, the Marcus theory is validated through an unconventional and robust approach based on conceptual density functional theory (CDFT).[6]

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EVOLVE: Integrating Statistical Mechanics and AI for Forecasting Protein Mutation

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Equilibrium Statistical Mechanics offers not only exact microscopic expressions for thermodynamic functions such as entropy and free energy, but also its most profound contribution—the fluctuation–dissipation theorem—relates spontaneous equilibrium fluctuations to the system's response under external perturbations. For instance, energy fluctuations relate to specific heat, volume fluctuations to compressibility, and number density fluctuations to susceptibility. These response functions often undergo daramatic changes or tend to diverge classifying phase transition onset and signaling critical phenomena. Landau theory provides a unifying framework to understand such critical phenomena, including recent extensions to *finite-time dynamical phase transitions* in far-from-equilibrium system. In the 1st part of my talk, I'll introduce the Mutational Response Function (MRF)**—**a statistical mechanics-inspired quantity that captures fluctuations in mutational entropy, serving as a dynamic quantitative marker to identify the emergence of SARS-CoV-2 *Variants of Concern* (VOC) and *Variants Under Monitoring* (VUM) as per WHO guidelines. Similar to dynamical phase transition, MRF exhibits sharp transitions that denote critical evolutionary crossovers, validated across viral genomes, transcriptomic, and proteomic datasets. The second part of the talk focuses on how mutational entropy reveals spatial mutational hotspots and functionally critical residues in viral proteins. Building on this, we present a statistical-mechanics-guided, ancestral-sequence-based machine learning framework to predict future domain-specific mutations with potential pathogenic implications. This integrative approach is implemented in **EVOLVE**—a publicly available web tool for mutation forecasting and sequence-space exploration (Figure 1), accessible at https://evolve-iiserkol.com.

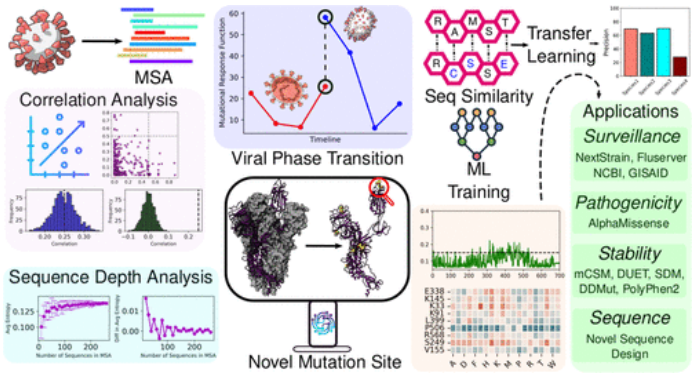


Figure 1: Sequence-Space Analysis through EVOLVE Webtool

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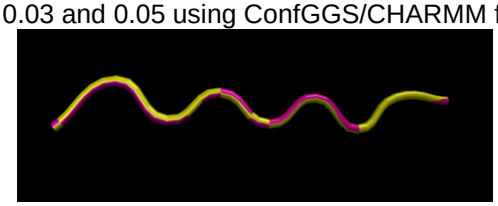
Computational Techniques in Drug Design: Emerging Trends & AI Integration

Prabhat K. Sahu

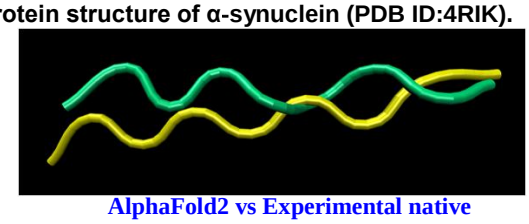
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Abstract

Computational techniques in drug design are taking center stage to mitigate the global challenges against different diseases. New and improved implementation of algorithms and adaptation of novel techniques[1,2] with available computational infrastructure, pave the way towards conformational search of proteins and to refine the design process of drug inhibitors. To overcome the drug-resistant strain is another aspect in designing the new inhibitors. The oral presentation will focus on the conformational search exploration using ConfGGS techniques using different force fields, advantages of CovDock, the state-of-the-art QM/MM approach towards inhibition mechanism. The computed MAE and MSD values are found to be 0.03 and 0.05 using ConfGGS/CHARMM for the **Protein structure of α-synuclein (PDB ID:4RIK).**

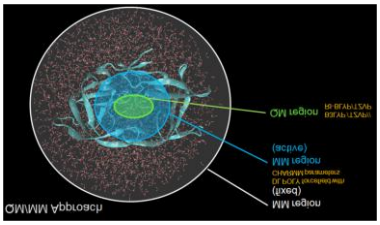


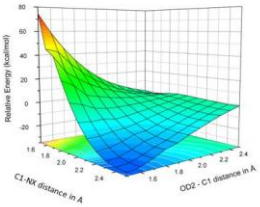
ConfGGS/CHARMM vs Experimental native



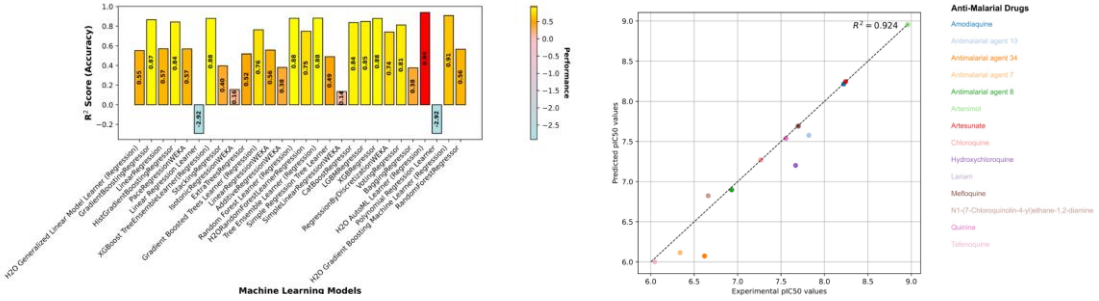
AlphaFold2 vs Experimental native

QM/MM Potential Energy Surface represent the inactivation process of HIV-1 PR (2SYH) through model Aziridine based inhibitor-1 (AZNP). The computed activation energy and the reaction energy are found to be 4 Kcal/mol and -36 Kcal/mol respectively.





Machine Learning exploration began with the creation of a virtual compound library, which was filtered using Lipinski's Rule of Five. Descriptor values were extracted via RDKit[3] from SMILES representations sourced from ChEMBL and PubChem. The refined dataset was analysed using 28 regression and 12 classification algorithms, with model performance validated against FDA-approved benchmarks with the R^2 value 0.924, as high accuracy.



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From Electronic Structure to Topology: AI-Guided Exploration of Iron-Based Molecular Complexes for Oxidation Reactions

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Non-heme Fe(IV)-oxo and their isoelectronic Fe(IV)-imido analogues are powerful oxidants central to C–H activation, alkene epoxidation, and nitrene transfer reactions. Computational studies elucidate the electronic factors governing their reactivity and can guide the design of next-generation catalytic complexes. [1] We have developed a computational framework that integrates quantum chemistry with machine learning (ML) to enable accurate and efficient screening of thousands of coordination environments. Central to this framework is a novel molecular fingerprinting method [2] based on persistent homology, an applied branch of algebraic topology, that captures geometric, electronic, and topological features of transition-metal complexes. [3] Using this approach, we have explored ligand effects on Fe(IV)-oxo sites by training ML models on high-level DFT data for a few hundred complexes to predict reactivity trends across large molecules databases. The resulting model identifies key descriptors controlling C-H activation and provides valuable design principles for new catalysts. [4] Ongoing work extends this methodology to Fe-tetracarbene complexes for epoxidation [5] and aziridination reactions. [6-8]

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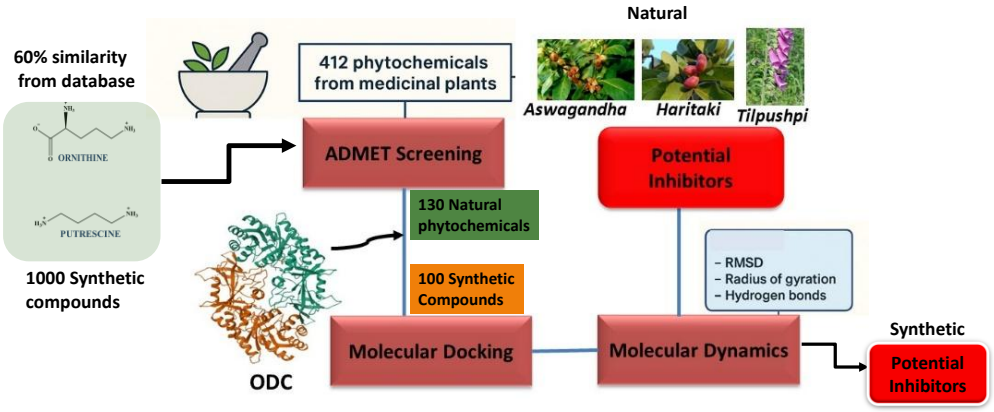
In Silico Screening of Natural and Synthetic Compounds as Potential Inhibitors of Tumor-Promoting Ornithine Decarboxylase

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Ornithine decarboxylase (ODC) is a pyridoxal-5′-phosphate-dependent enzyme central to polyamine biosynthesis and is often overexpressed in MYC-driven cancers, making it a valuable anticancer target. In this study, we employed a comprehensive Computer-Aided Drug Design (CADD) approach to identify both natural and synthetic ODC inhibitors and investigate their mechanistic interactions, including the role of water molecules in enzymatic inhibition. We first screened a curated library of 412 phytochemicals from 51 anticancer medicinal plants. Following drug-likeness and ADMET filtering, selected compounds were docked against the ODC homodimer. Top hits underwent 100 ns molecular dynamics (MD) simulations and MM-PBSA energy calculations, revealing five natural compounds with stable binding, favorable pharmacokinetics, and potential as reversible ODC inhibitors.

In parallel, ~500 synthetic analogs each of ornithine and putrescine (~60% similarity) were retrieved from chemical databases. ADMET screening narrowed these to 40–50 non-toxic candidates, which were subjected to docking and MD studies. Several synthetic molecules exhibited strong, stable interactions with the ODC active site.

Mechanistic analyses highlighted the critical role of structured water molecules in stabilizing ligand binding via hydrogen bonding networks, influencing inhibitor orientation and dynamics. This integrative pipeline combining natural compound discovery with synthetic analog screening reveals potent ODC inhibitors with promising pharmacological profiles. Our findings set the stage for experimental validation and further optimization toward selective anticancer therapies targeting polyamine biosynthesis.



Scheme 1 Screening methodology and identification of the natural/Synthetic compounds for ODC inhibition

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Modeling spin for applications of metal complexes

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Unpaired electrons are of importance for the reactivity of transition metal complexes and are responsible for spectroscopic and molecular magnetic properties of transition metal and rare earth compounds. Thorough quantum-chemical modeling combined with experimental studies help to optimize systems for specific applications. Three examples are presented to demonstrate the relation between coordination geometry and electronic structure: (i) The activation of oxygen by high-valent nonheme iron complexes, where the efficient modulation of the energy gap between the spin ground and first excited states lead to the most reactive iron(IV)oxido catalyst known todate.[1,2] (ii) A manganese(II) based MRI contrast agent with exceptional stability, manganese(II) selectivity and MRI efficiency.[3,4] (iii) The validation of ab-initio predicted magnetic anisotropies in dysprosium(III) compounds.[5-7]

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Theoretical Chemistry Symposium
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Dynamic Catalysis as a Novel Strategy For Efficient Chemical Transformations

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Dynamic catalysis is a phenomenon in which the catalytic properties of the system change with time. It has been recently proposed as an alternative to the current widely utilized static catalytic approach because of potential significant improvements in catalytic efficiency. Dynamic restructuring of active sites on surfaces has also been observed in some nanocatalysts. However, the microscopic mechanisms of underlying processes remain not well understood. We developed a new stochastic framework that allows us to quantitatively describe dynamic catalysis and compare its properties with the static approach.[1] It is found that fluctuations between different catalytic pathways might lead to enhancements in chemical reaction rates but only for specific ranges of kinetic parameters. Our theoretical method can explain these observations from the microscopic point of view. We show that the temporal efficiency of dynamic catalysis depends only on the rates of chemical reactions and transitions between different catalytic pathways while being independent of the number of active sites. It is also argued that the effects of dynamic catalysis are purely nonequilibrium, and the associated energy dissipation is the source of improvements in catalytic efficiency. The proposed theoretical approach clarifies some important microscopic aspects of catalytic processes.

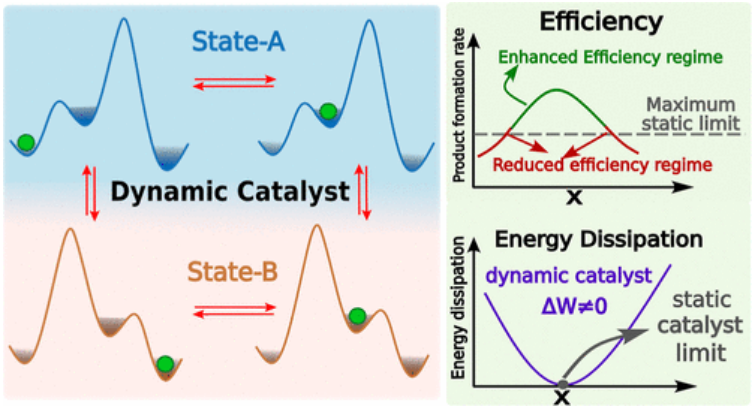


Figure 1 Schematic view of dynamic catalysis phenomena and their properties.

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New Developments Involving Graph Neural Network-based Algorithms for Structure Prediction and Global Optimization

Gunjan Ramteke, Sridatri Nandy and K.V. Jovan Jose

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Abstract: Understanding the evolutionary patterns and evaluating energies to determine the lowestenergy structures remains a long-standing challenge in computational studies of atomic and molecular clusters [1]. Accurately computing wavefunctions and associated electronic structure properties is highly demanding, requiring substantial time and computational resources. In recent decades, data-driven methods have become increasingly influential in probing chemical systems [2]. In this work, we introduce a data-driven Graph Neural Network approach capable of predicting molecular electrostatic potential (MESP) topographical minima to guide the design of metal clusters and their topology, thereby learning from molecular clusters [2,3]. We further exploit the directional nature of the MESP to generate stable, low-energy nanoclusters of various sizes through a global optimization algorithm. Benchmark results demonstrate that our method constructs and optimizes atomic clusters efficiently with minimal computational cost [4]. This talk presents our approach along with benchmark studies on prototype magnesium, calcium, and CO_2 clusters.

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Liquid State Integral Equation Theory to Study Biological Processes in complex ionic environments

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Ions play important roles in the function of biological systems. For instance, muscle contraction, neural signal transmission, RNA folding, and enzyme catalysis are some of the processes governed by specific ions. We have been investigating the role of ions in different biological processes using both molecular dynamics simulation and liquid state integral equation theory. In this talk, the selectivity of specific divalent ions in the activation of the motor protein Myosin will be discussed. The role of the Reference Interaction Site Model (RISM) methodology, a statistical mechanical theory, in calculating the ion density in the functional part of the Regulatory Light Chain (RLC) of Myosin will be illustrated.

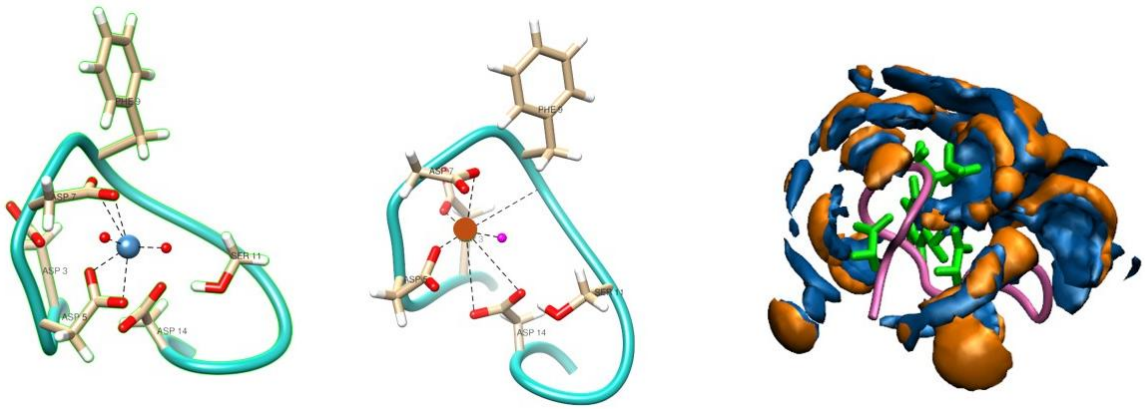


Figure 1: From left to right: RLC loops with Mg^{2+} and Ca^{2+} ion, density of divalent ions calculated with the RISM method. Blue is Mg^{2+} and orange is Ca^{2+}

Static vs dynamic rough energy landscapes: Where is diffusion faster?

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This turns out to be a trick question. Molecules in dense environments, such as biological cells, are subjected to forces that fluctuate both in time and in space. While spatial fluctuations are captured by Lifson-Jackson-Zwanzig's model of "diffusion in a rough potential", and temporal fluctuations are often viewed as leading to additional friction effects, a unified view where the environment fluctuates both in time and in space is currently lacking. I will describe a class of solvable models describing energy landscapes fluctuating both in time and in space. Importantly, these models account for the reciprocal interaction of the diffusing particle with the landscape, which alters the landscape dynamics. As a result we find, surprisingly, that many features of the observable dynamics do not depend on the temporal fluctuation timescales and are already captured by the model of diffusion in a rough potential, even though this assumes a static energy landscape. Using insights from this theory, I will revisit several experimental studies of biomolecular dynamics, in which the roughness energy scale was deduced from single-molecule measurements.

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Dynamical Origins of Stereoselectivity in the Thermal Deazetization of 2,3-diazabicyclo[2.2.1]hept-2-ene

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The thermal deazetization of 2,3-diazabicyclo[2.2.1]hept-2-ene (DBH) has been experimentally shown to favor formation of the exo-bicyclopentane (BCP**)** over the endo product. However, this stereochemical preference cannot be rationalized by static potential-energy analysis, which predicts a statistical 1:1 ratio of exo-BCP to endo-BCP due to degenerate transition states. To address this discrepancy, we performed *ab initio* classical trajectory simulations at the CASSCF level. The simulations reveal a predominant double-inversion pathway that is fully consistent with the experimental product distribution and show that the stereochemical outcome is governed by dynamic effects rather than energetic barriers alone. These results not only reconcile the experimental observations but also highlight the potential for dynamical matching to steer product formation in this reaction.

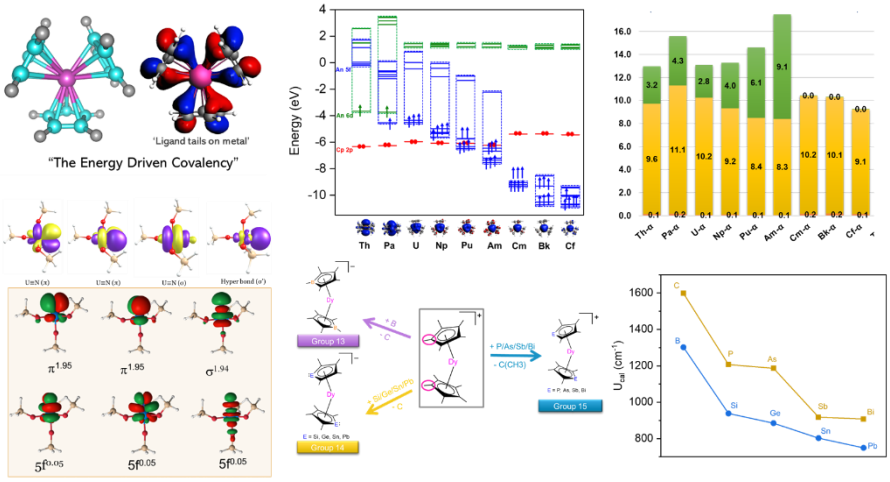
Theoretical Chemistry Symposium
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Correlating Electronic Structure, Covalency and Magnetic Anisotropy in f-elements

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The chemistry of lanthanides and actinides becomes fascinating due to their various technological applications1 in used nuclear fuel, waste repositories, designing molecule-based magnets for information storage applications, and catalytic applications for small molecule activations.[1] The complexity of the electronic structure stemming from their capacity to host electrons in the 5f/6d/7s/7p orbitals led to unique bonding motifs and chemical and spectroscopic properties, and hence understanding the nature of actinide-ligand bonding, covalency, and magnetic properties is a burgeoning research topic in the field of f-elements chemistry. The electronic structure and magnetic properties of 4f and 5f-based molecular complexes are challenging, and they require highly sophisticated relativistic quantum chemistry approaches within the DFT framework and multireference methods.[2] In the first part of my talk, I will describe the actinide-ligand covalency by analysing the orbital-driven components (role of 5f vs 6d orbitals), energy-driven covalency, nephelauxetic effects, and relativistic nephelauxetic effects in organometallic actinide complexes and the importance of metal-ligand covalency in precise calculations of the EPR parameters.[3-4] In the second part of my talk, the importance of lanthanide-ligand covalency and its correlation with magnetic anisotropy to design highly anisotropic lanthanide-based magnetic materials for information storage applications.[5-6]



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Spatiotemporal dynamics and emergent orders in chemical and biological systems

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In this talk, I will discuss our group's investigation into how externally applied electric fields influence pattern formation in reaction-diffusion systems containing ionic species. Using theoretical analysis and simulations, we explored a well-known experimental system-the photosensitive chlorine dioxide-iodine-malonic acid (CDIMA) model. Our findings reveal that electric fields induce diverse spatiotemporal patterns, including Turing-like stationary structures, moving spots, and wave-splitting phenomena, depending on the charge properties of reacting species. Additionally, I will briefly discuss the interplay between electric fields and periodic photo-illumination in the CDIMA system, leading to complex superposed patterns with hexagonal and square symmetries. These results open new avenues for experimental validation and the controlled manipulation of patterns in chemical systems.

I will also present our particle-based biophysical model exploring bacterial self-organization. Bacteria in natural environments exhibit collective phases such as swarms, patterned colonies, and biofilms, driven by growth, motility, and physicochemical interactions. Our model reveals how resource limitation and demographic fluctuations shapes the colony dynamics.

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Development of lead Molecules with Antiviral Properties using computational Tools

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Over the past two decades world has witnessed the infectious nature of the zoonotic viruses belonging to the coronavirus family, which is tremendously impact on the global economy. In the beginning of the 21st century, the deaths were mostly associated with SARS-CoV-1 and MERS-CoV. Due to their highly contagious nature, these viruses rapidly spread across the world, in march 2020 World Health Organization (WHO) declared SARS-CoV-2 as pandemic. It's crucial to advance the design and development of potent inhibitors for clinically used in the treatment of mild to severe infected patients. The efforts of the scientific community led to the rapid development of repurposed drugs during the pandemic to treat mild to severe cases, but still no targeted drugs for SARS-CoV-2. Spike protease and RNA-dependent RNA-polymerase RdRp are essential to viral entry and replication respectively, these are capable to develop as antiviral targets, however the Spike protein and RdRp has highly mutated in across the strains, makes challenging task to developing therapeutics against these targets. In contrast M protease (M^{Pro}) has emerging as an unsurpassed target, Mpro play a key role cleaving viral poly proteins (pp1a and pp1ab), which essential for viral replication. Notably the active site of Mpro is highly conserved among SARS-CoV-1, SARS-MERS and across different strains of SARS-CoV-2. Thus, design and developing inhibitors targeting Mpro provides tactic for develop broad-spectrum antiviral agents with potential efficacy against all SARS-Cov associated within the coronavirus family. Considering M^{Pro} as an effective target, we investigated natural products compounds to identify the potential inhibitors that binds to its catalytic site, thereby blocking polyproteins cleavage. We employed molecular docking for initial screening of Natural products followed by molecular dynamics for structural and conformation stability, enhanced sampling techniques MetaDynamics (MetaD) and Umbrella Sampling (US) Thermal Titration Molecular Dynamics (TTMD) for kinetic behaviour, MMPBSA/GBSA and Boltz2 for binding free energy uncertainties.

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HPE And Precision Infomatic

Bibhu Dash

How Photosynthesis Works: Insights from Multiscale Simulations

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Life relies on the ability of photosynthetic organisms to utilize sunlight for powering redox reactions. Photosystem II (PSII) is the enzyme responsible for the initial conversion of excitation energy into the flow of electrons that sustains all subsequent processes, as well as for catalysing the all-important oxidation of water into dioxygen. Primary charge separation takes place at the reaction centre of PSII, a unique assembly of strongly coupled chlorophyll pigments. The detailed electronic structure description of the reaction centre of PSII is essential for an atomic-level understanding of its function. This requires multiscale/multilevel simulations that incorporate methods able to tackle the structural complexity of the system, account for protein electrostatics, and perform reliably for excited states of pigment assemblies. Here I discuss advances in our understanding of the molecular mechanisms of photosynthesis obtained by multiscale (QM/MM) simulations with carefully optimized DFT and wave function based methodologies. These studies offer unprecedented atomic-level insights into the functional principles of photosynthesis, helping us to precisely identify the active pigments, characterise the primary charge-transfer states, and understand the crucial role of protein matrix electrostatics in generating the asymmetry and directionality that underlie the function of all photosystems.[1–7]

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Relativistic electronic structure calculations for spectroscopic properties of heavy-elemental compounds

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Relativity and electron correlation effects are necessary to accurately predict the electronic structure and properties of molecules containing heavy elements. Herein, we present the four-component relativistic electronic structure calculations of the properties relevant for high-precision spectroscopy and fundamental physics. Firstly, we have demonstrated the application of the relativistic coupled-cluster (RCC) method to compute the symmetry violating properties in a ultracold polyatomic system, SrOH, as a test case, which can be employed for other heavy ultracold polyatomic systems such as BaOH, YbOH, RaOH, etc. Furthermore, we assess the reliability of the fully relativistic density functional theory for accurately calculating the hyperfine structure coupling constants of heavy molecules by comparing with the results evaluated through the RCC method.

Classical Trajectory Simulations of Gas Phase S_N2 Reactions

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Gas-phase dynamics of bimolecular nucleophilic substitution (S_N2) reactions have long been a focal point of both experimental and theoretical research, owing to their broad relevance and the continual emergence of new mechanistic insights. Extending such studies to larger nucleophiles is essential for bridging fundamental model systems with more complex organic chemistry. In this talk, I will present classical trajectory simulations of two prototypical S_N2 reactions -- $CH_3I + CN^-$ and $CH_3I + CH_3O^-$. Both reactions have been previously investigated using velocity-map imaging (VMI) experiments, which revealed several intriguing dynamical features. Our simulations offer a detailed, atomistic-level view of these processes, uncovering distinctive mechanistic pathways and product branching ratios across their multiple reactive channels. The required potentials and gradients for the trajectory integrations were obtained either through *on-the-fly* direct dynamics or by constructing a neural-network-based analytical potential energy surface. The simulation outcomes show strong agreement with experimental observations and provide deeper insights into the complex dynamics that govern these benchmark S_N2 systems.

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The Hidden Choreography of Ions in Acid-Base Chemistry: A Constant pH MD Perspective

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The modulation of acid-base equilibria by salts is a cornerstone of solution chemistry, yet the underlying mechanisms in complex, multi-component electrolyte mixtures remain poorly understood. While prior studies have established that individual salts can induce ion-specific shifts in the pKa of weak acids, the molecular origins of these effects have not been systematically elucidated.

In this talk, I will discuss how ion pairing influences amino acid deprotonation equilibria. Using constant pH molecular dynamics simulations, we recently uncovered that cations and anions modulate acid-base equilibria through fundamentally distinct mechanisms governed by their relative affinities, and those of the acid, for water.[1] Furthermore, a simple coarse-grained model is introduced for investigating the pH-dependent collapse of hydrophobic polymers,[2] providing a computationally efficient approach to studying acid-base equilibria and charge regulation effects in interfacial soft matter and biomolecular systems.

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Vibronic Quantum Algorithms for Spectroscopy and Dynamics

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Quasiparticles such as polarons, bipolarons, and excitons play a central role in determining the electronic, optical, and transport properties of molecular aggregates, thin films and crystals, and semiconducting polymers. In such π-conjugated systems, charged (polarons) and neutral (excitons) excitations are strongly coupled to nuclear degrees of freedom, underscoring the importance of electron–phonon interactions. We will explore how similarly structured Holstein-style non-adiabatic vibronic Hamiltonians can be constructed to probe the spectroscopy and dynamics of a broad range of quasiparticles, including polarons,[1] bipolarons,[2] and excitons,[3] for applications in energy and charge transport, optoelectronics, and quantum information sciences.

A theory will be presented that describes the spatial coherence length of polarons[3] in disordered organic materials, revealing a simple relationship between the oscillator strength of the infrared absorption band and the polaron coherence function. Holstein-style theoretical frameworks, represented in a multiparticle basis set, have been highly successful in quantitatively reproducing several recently measured spectra recorded in doped and undoped polymer films, confirming the association between enhanced peak ratios and extended polaron coherence. Emphasis will be placed on understanding the fundamental nature and origin of components polarized along the intra- and inter-chain directions and their dependence on structural and conformational disorder, vibronic coupling, and Coulomb binding.

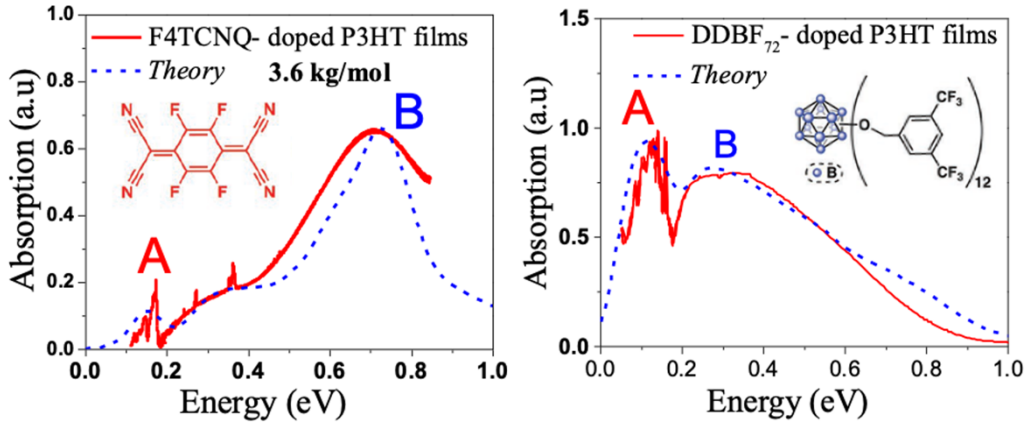


Figure 1: Comparison of Holstein Hamiltonian–based simulations with infrared measurements of polarons in chemically doped organic materials.

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The Interesting Chemistry Talk

Dr. Muthukumar Kaliappan

Applied Materials Inc, Santa Clara, CA, USA

Chemistry underpins the technology we use daily, from smartphones to supercomputers. In this talk, Dr. Muthukumar Kaliappan examines how chemical modeling and machine learning intersect to advance electronic device innovation. The presentation highlights molecular-level engineering and interdisciplinary strategies shaping the future of electronics.

About the Speaker:

Dr. Muthukumar Kaliappan is a senior scientist at Applied Materials with over 20+ years of experience in modeling and simulation. His work focuses on developing next-generation technologies through a deep understanding of materials and chemistry. Known for making complex science approachable—entertaining—and occasionally classified.

Shedding light on the Mechanism of Metal-free, Ultrafast Activation & Functionalisation of C-H bonds exploiting Photo Induced Charge-Transfer in Host-Guest systems

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C-H activation under ambient conditions invariably involves transition metal catalysts. However, on rare instances it has been shown experimentally that C-H activation of hydrocarbons and subsequent oxidation can be facilitated by encapsulating an organic substrate in a host cage molecule followed by photo induced charge transfer (PET) from the incarcerated species to the captor host [1-3]. Such oxidation of hydrocarbons has been achieved in metal containing [1. 2] as well as metal free cages [3]. Unfortunately, the mechanism of such oxidation processes remains elusive till date. This talk would focus on our findings on from theoretical investigations of the Proton Coupled Electron Transfer (PCET) processes which are triggered on Photoexcitation followed by reaction with $^3O_2$ ultimately leading to the oxidized product.

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Theoretical Chemistry Symposium
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On the interplay between metal-metal and metal-ligand bonding in Zintl clusters: complementary perspectives from DFT and MC-SCF

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Endohedral clusters present a fascinating challenge to theories of chemical bonding, simply because the nature of the interaction between the endohedral atom (or atoms) and the cage can vary from van-der-Waals'-like to strongly covalent. In the former case, the endohedral atom is held inside the cage only by the barrier to passing through the wall, whereas in the latter, charge transfer can influence the structure of the cage. In clusters with two or more endohedral metals, the situation is further complicated by the potential for metal-metal bonding, and the interplay between this and metal-cage bonding leads to a complex electronic landscape. In this presentation, I will discuss our latest work using both DFT and MC-SCF approaches, which give different but complementary perspectives on the nature of chemical bonding in this fascinating class of clusters.[1,2]

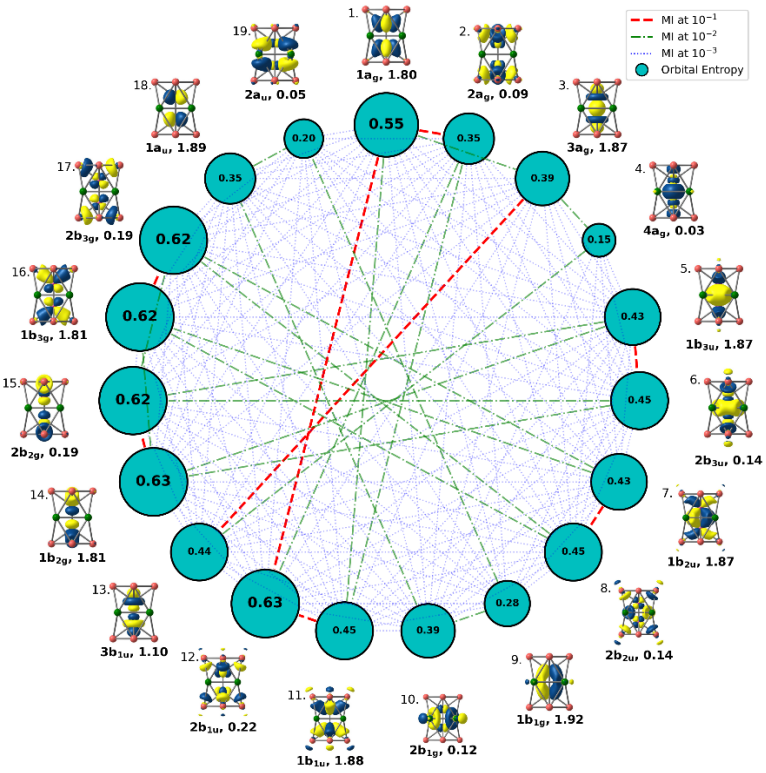


Figure 1 Orbital entanglement in $[Fe_2Sn_4Bi_8]^{3-}$.

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AMD

Sudhakar Yerneni

Engineering power conversion efficiency of porphyrin sensitizers for DSSC through metal, ligand and bridge modification: a DFT study

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Systematic investigation of porphyrin sensitizers for application in dye-sensitized solar cells (DSSCs) has been performed using static and time-dependent density functional methods. The well-established SM315 dye, known for its record-breaking PCE of 13%, was adopted as a reference point. A range of metal atoms including alkaline-earth and 3d transition metals were screened, Ca was identified as the most promising metal for light capture and conversion. Ca–porphyrin-based sensitizer was further modified by introducing different axial ligands and distinct bridging units. The performance of the in silico designed photosensitizer was evaluated in an operational solar cell setup with a TiO_2 semiconductor and I_3^-/I^- electrolyte. The designed dyes exhibit red-shifted absorption spectra and optimal frontier orbital alignment with the semiconductor's conduction band, promoting efficient light capture and charge transfer. A comprehensive analysis of parameters like light harvesting efficiency , reorganization energy, short-circuit current density, exciton binding energy, open-circuit voltage, electron transfer rate, polarization and hyperpolarization collectively paint a clear picture of superior light capture, efficient charge transport dynamics, and minimized energy losses within the designed dyes. This ultimately translates to the remarkable power conversion efficiency surpassing the performance of SM315 dye (13% PCE). This systematic study combines the design of high-performance porphyrin sensitizers through molecular engineering with a comprehensive investigation of their impact on DSSC function using advanced computational methods.

Mechanistic understanding on the potential of graphene-based nanoflakes in inhibiting the $A\beta_{42}$ aggregation.

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The accumulation of fibrillar amyloid-β (Aβ) peptides is a central pathological feature in Alzheimer's disease (AD). Disrupting the formation of amyloid fibrils and β-sheet structures is a pivotal therapeutic strategy for AD treatment. Graphene oxide has received significant research interest as a potential inhibitor of Aβ aggregation, owing to its unique structural attributes, exceptional physical properties, and ability to cross biological membranes. Recent in vitro investigations have emphasized the substantial research interest in graphene oxide nanoflakes (GO) and their potential to inhibit $A\beta_{42}$ aggregation. However, the mechanism underlying the interaction between $A\beta_{42}$ and GO nanoflakes, as well as the inhibitory effect on molecular-level aggregation, remains unclear. In this study, we investigated the structural characteristics of the $A\beta_{42}$ in the presence of pristine graphene, GO, and reduced graphene oxide (RG) nanoflakes of different sizes through molecular dynamics (MD) simulations and simulated annealing approaches. Our study demonstrates a substantial decrease in β-sheet content and hydrogen bonding of $A\beta_{42}$, accompanied by enhanced electrostatic and Van der Waals interactions of $A\beta_{42}$ with GO and RG nanoflakes, which play a significant role in inhibiting the aggregation of the amyloid peptide. The order of interaction of graphene nanoflakes with $A\beta_{42}$ was found to be G < GO < RG. Apart from the functionalization, the surface area of the nanoflakes also plays a crucial role in disaggregating or inhibiting $A\beta_{42}$, where larger-sized nanoflakes, such as RG5, are found to be more effective compared to their smaller-sized counterparts. The structural mechanisms by which GO and RG nanoflakes inhibit $A\beta_{42}$ aggregation are elucidated in this study, findings that are useful for the development of innovative therapeutic interventions for AD.

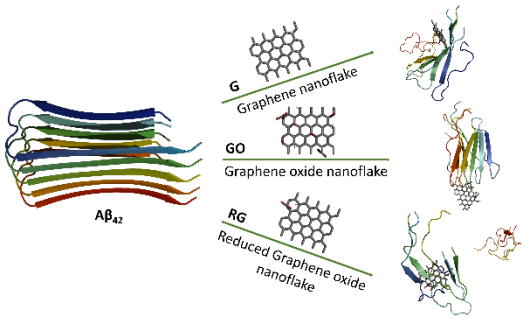


Figure 1: Graphene-based nanoflakes in inhibiting the $A\beta_{42}$ aggregation**.**

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Theoretical Chemistry Symposium
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Insights into Transport in Aggregates: Path Integral Approaches

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Transport in molecular aggregates is a problem of dynamics in many-body systems. Simulations are complicated by the presence of a vibrational manifold of states that are thermally populated and which interact non-perturbatively with the electronic degrees of freedom. These environmental degrees of freedom can often be extremely complicated like the impact of protein scaffoldings on the dynamics of photosynthetic excitonic transport. Path integrals with the Feynman-Vernon influence functional[1] provide a lucrative method for simulating the excitonic dynamics in these systems. In our group, we have been working on developing methods that make simulations of these complicated systems even involving other processes[2] more efficient and taking steps towards understanding the dynamics in these molecular and polaritonic aggregates in greater detail. Generally molecular aggregates that occur in nature have complicated geometries and non-trivial inter-monomer couplings. So the excitation from one molecule has a probability of hopping to multiple other molecules. How does one then understand the routes of transport of the excitation from its initial position using the time-evolution of the excitonic density matrix while ensuring that the vibrations, solvents, and effect of potential protein scaffolding are treated exactly? We will show that surprisingly it is indeed possible to extract this information from the many-body dynamics.[3,4] These methods have now been extended to handle cases when there is a loss of the exciton from the system described by a non-Hermitian term in the Hamiltonian, as would happen in transport aggregates, allowing us to talk about the emergent efficiencies of transport specific to end-points when the aggregate has multiple end-points.[5] A combination of these analysis methods along with the new simulation methods being developed both in our group and others promises to be crucial to elucidating quantum transport in complex open quantum systems.

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Unraveling Intracellular Protein Phase Separation with Minimal Models

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Liquid-liquid phase separation of biopolymers, such as proteins and RNAs, is now widely recognized as a vital phenomenon driving the formation of biomolecular condensates in living cells. These condensates are integral to a wide range of cellular processes, and therefore, understanding the physical principles underlying the intracellular LLPS is essential for insights into aging and various human diseases. As a consequence, there is now a growing interest in developing rational design strategies for protein sequences that exhibit thermo- or stimulus-responsive phase behavior, with potential applications in synthetic biology. However, despite extensive experimental and computational efforts over the past decade, mechanistic understanding of condensate morphology selection and its interplay with solvent and external environmental conditions remains limited. A part of the challenge lies in probing the solvent and/or stimulus-induced changes in protein conformations and establishing a direct connection between stimulus-driven changes in protein internal conformational states and the resulting changes in solvent-mediated effective inter-protein interactions. In this talk, we shall present minimal statistical mechanical models based on the Lattice-Gas Hamiltonian which explicitly accounts for the protein's internal conformational state dependent inter-particle interaction to probe their roles in condensed morphology selection [1,2]. We shall further discuss the anomalous re-entrant and wetting-mediated phase separations (for the case of two-component mixtures) and the influence of non-equilibrium conditions on the phase behavior and stability of biomolecular condensates. Our framework aims to provide mechanistic insight and guide the rational design of protein sequences and environmental conditions for targeted control of condensate morphology.

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Non radiative decay processes in weakly bound systems

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We will discuss the decay mechanisms that follow ionization of inner-valence states, focusing on ionized alkali metals (Li^+, Na^+, K^+) that are micro-solvated by water molecules [1-4]. We examine the key factors that influence the lifetime of these decaying states and highlight the specific role played by water molecules in shaping the decay pathways. Additionally, we explore how the preferred mode of decay varies among different alkali-metal ions and how micro-solvation modifies these processes[2,3]. The influence of environmental factors—including polarization effects, molecular geometry, and pH—on the decay dynamics of these systems.

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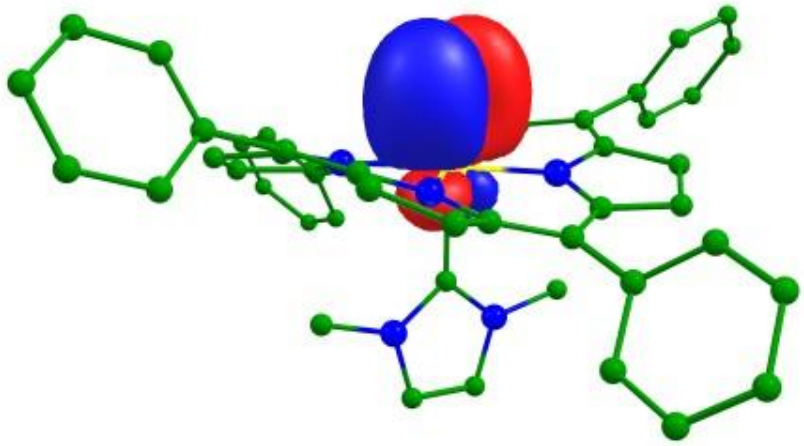
Understanding the Reactivity Trend of High Valent Metal-oxo Species towards C-H Activation

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Oxygenated metal intermediates are involved in the reaction mechanism of mononuclear metalloenzymes such as oxo, peroxo, hydroperoxo and superoxo species to gain ample attention in the field of bioinorganic chemistry.[1-6] In the past decades, these bio-mimetic complexes have been synthesized and several high-valent metal-oxo/hydroxo complexes are spectroscopically detected and for some even X-ray structures are available, their catalytic selectivity, efficiency and robustness are diverse. In this presentation, we will discuss our research efforts to underpin the reactivity trend and mechanistic insights into C-H Bond activation and oxygen atom transfer by high-valent transition metal-oxo complexes.



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Machine Learning and Multiscale Modeling Approaches in Molecular Simulations

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Recent advances in Machine Learning (ML) and data-driven methods are transforming molecular simulations. While traditional molecular dynamics techniques are powerful, they are often constrained by force field accuracy and the timescales they can access. ML-based interatomic potentials (MLIPs) provide quantum-level accuracy at near-classical computational cost, expanding the predictive capabilities of simulations, while enhanced sampling simulations with data-driven collective variables accelerate the exploration of complex free-energy landscapes within affordable computational expense. Furthermore, multiscale modeling approaches, particularly coarse-grained models, enable the simulations of large macromolecular complexes. In this talk, I will present our recent work on developing data-efficient MLIPs for studying phase transitions, gas diffusion in framework solids, and catalysis. The second part will highlight our recently-developed graph-coarsening–based coarse-grained modeling approach and its applications to complex molecular systems. These methodologies are general and versatile, offering pathways to simulate a wide range of systems and physicochemical processes.

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Nvidia
Manish Modani

Vibrational Spectroscopy Modeling to Study Aqueous Systems

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The presence of external solute alters the local structures and dynamics of water. The nature and extent of these structural modifications depend on several factors. Particularly, the chemical nature of the solute is very crucial. Theoretical spectroscopy can serve as a more powerful tool where spectroscopic data cannot provide the microscopic picture. In this talk, we will highlight a theoretical spectroscopic map based on a hybrid quantum–classical molecular simulation approach and discuss its applications in understanding the microscopic properties of several aqueous systems. Initially, we will highlight how the hydrophobic solute methane modulates the local water structure in its solvation shell and what the length scale for such perturbation is. In the second example, we will discuss the microscopic solvation structure of TMAO in water using five different classical force fields for TMAO and ultimately identify the best force field. Finally, we will discuss the urea-water scenario. We will first identify the best classical force field among the most popular force fields of urea, and finally identify the reason why urea does not perturb the water spectroscopic signature at all, even at higher concentrations.

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Remembering Seymour Cray: Architect & Builder of Supercomputers

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This year marks the 100th anniversary of Seymour Cray's birth (September 28, 1925) in Chippewa Falls, Wisconsin USA. After high school, Cray served in the US Army in WWII. First, he was a radio operator in Europe, participating in the '***Battle of the Bulge***' during the winter 1944 / 1945. Next, he was transferred to the Pacific theatre, where he worked on breaking Japanese naval codes. After WWII, Cray attended the University of Minnesota and graduated with a degree in electrical engineering in 1950. While pursuing a master's degree in mathematics, Cray joined ***Engineering Research Associates*** (ERA) and began designing computers, notably contributing to the UNIVAC 1103. In 1958, Cray left ERA to join other former ERA colleagues, who had created the ***Control Data Corporation*** (CDC). There, Cray led the design of the CDC 1604, one of the first computers to use transistors. Later he helped create the iconic CDC 3600, as well as the CDC 6600 & 7600 computers. The CDC 6600 debuted in 1964 as the world's fastest computer. Cray left CDC in 1972 and created ***Cray Research Inc.***, which delivered the first Cray-1 supercomputer to LANL in 1976. Other supercomputers, e.g., the X-MP, Y-MP, etc., were delivered in the 1980s. Seymour Cray died, from injuries suffered from an automobile accident, in 1996.

My talk will briefly review the early history of computers, starting from the creation of electromechanical machines, and electronic vacuum-tube computers. I will then transition to the advent of commercial transistor-based computers, highlighting the pioneering contributions of Seymour Cray. Notably, 50-years after the announcement of the CRAY-1, in 1975, the name CRAY remains synonymous with the world's fastest supercomputers.



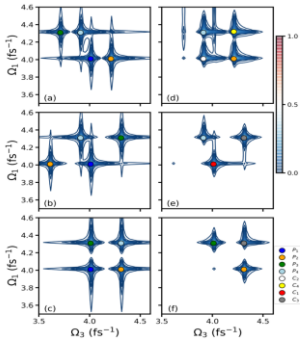
Figure 1. Seymour Roger Cray (September 28, 1925 - October 05, 1996)

Spectroscopy with quantum light

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Quantum entanglement correlates two or more particles in a non-classical way. Time-frequency entangled photon field, also known as quantum light, has been proposed [1] to utilize in optical spectroscopy to gain insights into the chemical dynamics of molecules with resolutions that is not possible with classical light. The hope is to use entanglement as an extra control knob to study molecular dynamics in the regime not possible with classical light. Nonetheless, this advantage with quantum light is not without its trade-offs.

It is difficult to observe signals generated using quantum light. Even at moderate field intensities, the molecular response is dominated by the interactions with photons that are not entangled leading to “classical” signal that can easily mask the quantum features. At sufficiently low-intensities where quantum features are supposed to be dominating, the signal is extremely difficult to observe and has been controversial [2]. In this talk, I shall present results for two-photon absorption [3] and 2-dimensional electron-vibration spectroscopic [4,5] signals using quantum light, discuss some advantages, and propose simple schemes to improve the quantum signal by removing the “classical” signal at higher field intensities.



Frequency-dispersed 2D electronic spectra using quantum light. Classical (a-c) and quantum (d-f) components to excited-state absorption (top), emission (middle), and ground-state bleach signals. Colored peaks are for population (P) and coherences (C)[Ref. 5].

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Relativistic Real-Time DFT: Probing Light-Induced Ultrafast Phenomena

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Recent advances in laser technology enable to track electronic motion on its natural timescale using ultrafast pulses, paving the way for atto- and femtosecond spectroscopic experiments. Understanding these laser-driven processes involves nonlinear light–matter interactions and nonequilibrium electron dynamics. Real-time electronic structure methods offer a direct route to simulating experiments and gaining insight into these processes.

In this presentation, we showcase the capabilities of relativistic real-time electron dynamics density functional theory combined with exact two-component (X2C) Hamiltonian models[1,2], as implemented in our ReSpect program[3]. Using this framework, we illustrate a series of interesting light-induced ultrafast phenomena, from charge and current density migration to the emergence of electronic chirality in oriented achiral molecules[4,5]. To unravel the underlying mechanisms, we further introduce a user-friendly visualization studio that transforms complex dynamical data into clear physical insight[6].

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Criterion to Characterize Non-Covalent Interactions and Their Cooparativity

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Chemical bonds are central to our understanding on the formation of moleculs, their aggregation and matter. While covalent bonds are very rigorously studied and characterized, the subtle nature of non-covalent interactions escape the attention to detail and are generally considered as weak interactions. Traditionally, hydrogen bonding and van der Waals interactions are synonymous with non-covalent intreactions. Here in this talk, I would like to discuss a rigorous criterion to characterize chemical bonds, their cooperativity, as well as the variety of non-covalent interactions which are being explored in recent years. Some examples on the manifestation of these non-covalent interactions in controlling the structure, stability and function of proteins and protein-protein inteactions.

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Computational design of stimuli-responsive biopolymer-grafted nanoparticles for therapeutics

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Polymer grafted nanoparticles are hybrid materials where the organic or inorganic nanoparticles are functionalized with biopolymers of desired chemistry.[1,2] These biopolymers can be biomolecules such as DNA, proteins or can be stimuli-reponsive synthetic polymers. These hybrid materials find attractive applications in biodiagnostics and therapeutics. We have worked on designing these grafted nanoparticles in an aqueous environment such as that found inside a crowded living cell to mimic the solution milieu that these nanoparticles encounter in biological fluid once administered into the patients.[3-5] Using molecular dynamics simulations, we have designed ss-DNA functionalized gold nanoparticles in molecular crowded environment of mixed amino acid solutions. Examining the solvation thermodynamics indicates that the solvation free energy of these nanoparticles is dependent on the effective size of the nanoparticles, which in turn is determined by the chemistry of the molecular crowders.[6] The ss-DNA sequence dependent change in the effective size of the nanoparticles is observed. We have also designed generic polymer-capped nanoparticles that are responsive to the change in temperature. By tuning the hydrophobicity of these polymers, a similar response to the size of the nanoparticles is observed as found by varying the temperature. Furthermore, thermo-sensitive gold nanoparticles have also been designed that are capped with PNIPAM (Poly-N,N'-isopropylacrylamide) chains. The competition between polymer collapse transition and polymer-nanoparticle interactions determines the overall effective size of the nanoparticle in presence of temperature stimulus. The talk will disucss the microscopic view of the effects of molecular crowding, hydration and biopolymer chain chemistry on the structure, stability and stimuli-response of grafted nanoparticles.

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Mechanistic Aspects of SWCNT Dispersion in RTILs

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Imidazolium based ionic liquids were found to be a signicant dispersing agent for Carbon Nanotube (CNT) bundles. In this report, we have conducted Molecular Dynamics (MD) simulations followed up with DFT based analysis, for investigation of the mechanistic details of SWCNT dispersion interaction in ionic liquids. Free energy change associated with dispersion obtained from umbrella sampling simulations revealed that the 1-Butyl-3-methylimidazolium tetrafluoroborate (BMIM BF_4) is the most potent Room Temperature Ionic Liquid (RTIL) for SWCNT dispersion, among four dierent imidazolium-based ionic liquids. However, the underlying molecular interactions were not obvious. Consequently, we performed quantum mechanical calculations on the simulated structures. All the calculations suggest that the associated anion determines the availability of the imidazolium ring of the BMIM cation near CNT surface. Our report provides detailed insights into the stabilization mechanism of imidazolium-based room temperature ionic liquids at the surface of SWCNTs as well as its dispersion.

Quantum Dynamics of Chemical Systems of Astrophysical Interest

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Abstract:

Astroplysical environment is composed of a galaxy of molecular systems of wide variety. It ranges from diatomics to polyatomics. In this presentation I will discuss on quantum dynamics of some of them both in particular, focusing on large molecular systems. For the purpose I will discuss on vibronic dynamics of linear carbon chains [] and Renner-Teller effect studied in our group in the recent past. Multi-dimensional potential energy surfaces with multiple conical interactions are developed for all of them. The quantum dynamics is studied in the multidimensional Hilbert space. Theoretical results are compared with experimental findings.

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Why Variational Density Functional Theory Is More Accurate Than Time-Dependent Density Functional Theory for Certain "Difficult" Excited States?

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Despite its remarkable success across a wide variety of excited states, time-dependent density functional theory (TDDFT) can fail severely for specific types of systems- for example, charge-transfer excited states[1], inverted singlet-triplet molecules[2], core excitations[3], and others. On the other hand, variational excited-state density functional theory (eDFT) performs comparably to TDDFT for "well-behaved" systems but consistently outperforms it for difficult excited states where TDDFT yields significant errors or incorrect qualitative results. In this talk, the energy equations of eDFT will be compared with a two-state model of Tamm-Dancoff approximation (TDA) TDDFT in order to investigate the origins of both the successes and failures of these two methods for three problematic classes of excitations- core excitations, inverted singlet-triplet molecules, and intermolecular charge-transfer excitations. A general decomposition framework will be presented for singlet and triplet excitation energies computed using eDFT and TDDFT, enabling analysis of how different exchange–correlation functionals contribute to orbital energy differences, kernel effects, and orbital relaxation. This analysis highlights the critical importance of selecting both the appropriate excited-state method and the functional in order to achieve reliable excitation energies.

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Dark Light, Smart Design: Cracking the Code of NIR-TADF with ML-Guided Inverse Design

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Designing efficient thermally activated delayed fluorescence (TADF) emitters in the near-infrared (NIR) region remains a formidable challenge due to the energy-gap law and non-radiative losses. In this work, we present a machine learning–guided inverse design strategy that integrates structural insights from non-fullerene acceptors and known TADF materials. Using interpretable models and fragment-based molecular generation, we discover novel hybrid emitters with verified NIR emission (up to 1359 nm) and favorable photophysical properties. Our approach expands the TADF chemical space, offering a scalable path toward next-generation organic materials for optoelectronic and bioimaging applications.

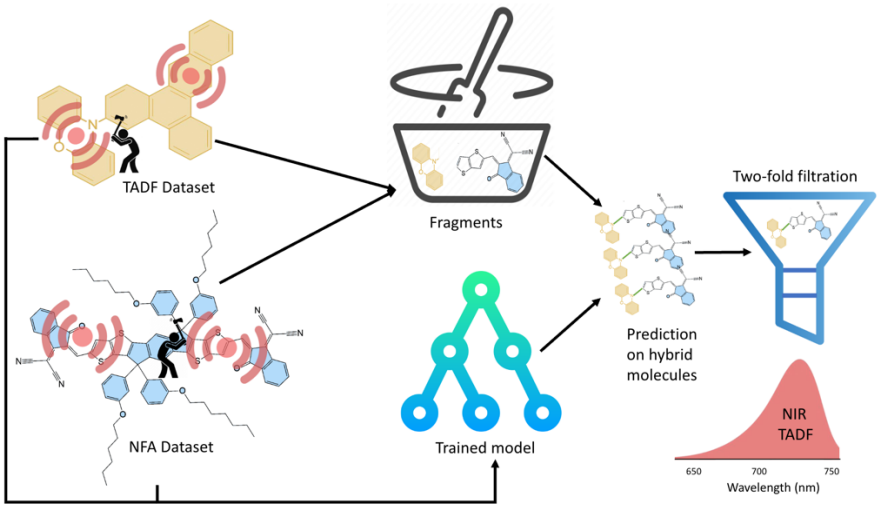


Figure 1 Schematic workflow of the ML-guided inverse design framework developed in this study. The process integrates curated datasets of non-fullerene acceptors and TADF emitters, feature extraction and model training, identification of NIR-enhancing fragments via model interpretability, and generation of novel NIR-TADF candidates. Top-ranked molecules are further validated through experimental synthesis and photophysical characterization.

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Thermodynamic principles for regulating of H-atom abstraction reactivity

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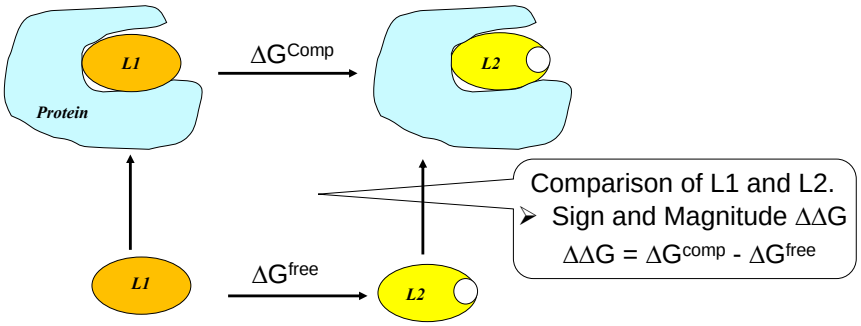
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Recently, we have formulated a concept going beyond the traditional relationship between thermodynamics and kinetics, which includes the effect of off-diagonal thermodynamics on reactivity. Here, I will present the latest advances in the concept. Among others, this will cover Marcus cross relation enhanced by asynchronicity. Also, I will show a hydride-coupled electron transfer (HCET) as a fundamentally distinct mechanism alternative to proton-coupled electron transfer (PCET) and show how this is pre-determined by off-diagonal thermodynamics. If time allows, I will also explore additional aspects of the concept, including how the asynchronicity of H-atom abstraction (HAA) process may influence the product outcome—particularly in cases where HAA gives rise to multiple post-HAA reactive pathways with low or negligible kinetic barriers.

Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

When Molecules Meet: MD Simulations Illuminate Biomolecular Recognition

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Molecular dynamics free-energy calculations quantify the strength of biomolecular interactions and reveal how structural features drive preferential binding, providing a rigorous framework for understanding molecular recognition. This talk will highlight how alchemical free-energy simulations advance the rational design of potent antimicrobial peptides (AMPs) and illuminate key aspects of the Cas9 genome-editing.[1-6]

AMPs offer a promising alternative to conventional antibiotics due to their broad-spectrum activity and lower rates of resistance, yet the mechanisms governing their interactions with bacterial membranes remain poorly defined, complicating rational design. Cas9, an RNA-guided nuclease widely used for genome editing, requires a specific protospacer adjacent motif (PAM) to initiate DNA recognition. This dependence narrows the range of editable sequences. Although certain mutations relax PAM specificity, the energetic basis of altered recognition and its relationship to atomic structure remain unclear. As a result, the development of new AMPs or engineered Cas9 variants often relies on empirical screening, a process that is time-consuming and resource-intensive.

To address these challenges, we examine the changes in binding affinity between peptides and membrane-mimetic models, which guide the design of more effective antimicrobial agents. Using free-energy calculations, we designed and synthesised small cationic peptides with potent, broad-spectrum activity against multiple ESKAPE pathogens and fungal strains.[1,4-6] Likewise, computed changes in DNA binding affinity for Cas9 mutants provide structural and energetic explanations for observed cleavage activity.[2-3] We propose minimally mutated Cas9 variants predicted to retain cleavage capability, pending experimental validation. Overall, molecular dynamics free-energy calculations clarify existing experimental data by connecting structure, energetics, and activity, while generating testable hypotheses for future investigation.

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Theoretical Chemistry Symposium
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Tuning the reactivity of Mn^{III}-O_2/OOH species in catalytic oxidation reactions: A DFT study

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In recent years, the field of bioinorganic chemistry has increasingly focused on the development of non-heme metal complexes for dioxygen activation and their application in a wide range of oxidation reactions under mild conditions. During dioxygen activation, mononuclear non-heme metal–oxo species such as M^{III}–peroxo, –superoxo, –hydroperoxo, and $M^{IV/V}$–oxo intermediates are typically generated and serve as reactive species in selective oxidation processes leading to alcohols, epoxides, sulfoxides, and related products. Elucidating the structures and reactivity of these intermediates has therefore been a major area of research. In this study, TMC-based Mn complexes are explored using DFT methods to evaluate their catalytic performance in sulfoxidation and epoxidation reactions. For sulfoxidation, the catalytic efficacy of two potential oxidants, Mn^{III}–OOH and Mn^{III}–O_2, was investigated.[1] The results reveal that Mn^{III}–OOH exhibits higher activity than Mn^{III}–O_2 by +16.6 kcal/mol. Interestingly, tuning the Mn^{III}–O_2 species through the incorporation of non-redox metal ions (M^{n+} = Sc^{3+}, Y^{3+}, Mg^{2+} and Zn^{2+}) enhances its sulfoxidation reactivity, making it comparable to Mn^{III}–OOH. For epoxidation, the role of additives (*eg.* -OAc, -OH and -HSO_4) was examined in modulating the catalytic activity of Mn^{III}–OOH.[2] The additive promotes the generation of high-valent Mn^{IV}–$O^{\bullet}$/Mn^{V}–O species, which in turn facilitates efficient epoxidation of alkenes. Overall, our findings highlight the strategies for tuning the catalytic activity of non-heme Mn–oxo species, thereby expanding their potential in diverse catalytic applications.

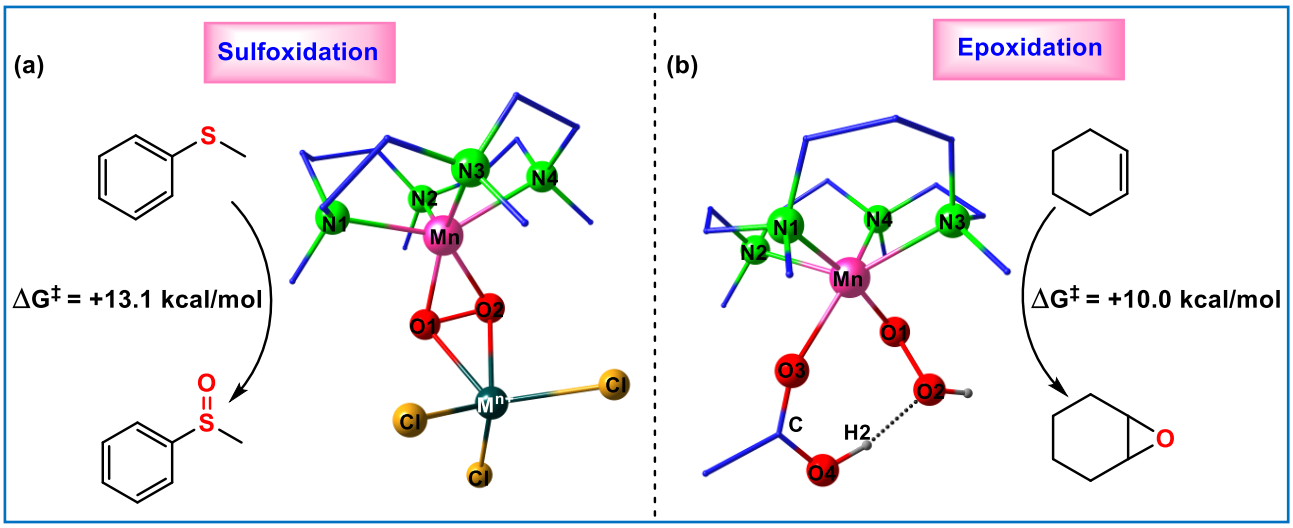


Figure 1. Tuning the catalytic activity of [Mn^{III}(13-TMC)(O_2/OOH)] complexes for efficient (a) sulfoxiation and (b) epoxidation reactions.

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Three irons on a sombrero: vibronic acrobatics and magnetic marvels on a Mexican hat

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Polynuclear transition-metal complexes with triangular metal arrangements are prototypical systems for investigating magnetic exchange, spin frustration, and symmetry breaking in molecular magnetism. In particular, μ_3-oxo-bridged Fe_3 spin triangles display rich magnetic behavior with implications for single-molecule magnetism and its control by the electric field. In the ideal equilateral case with C_3 symmetry, isotropic antiferromagnetic exchange among the three Fe(III) centers produces a doubly degenerate $|^2E\rangle$ ground state, directly reflecting the frustrated topology. To interpret the experimental findings, deviations from perfect symmetry are claimed, and magnetic susceptibility and EPR data require two exchange parameters (*J*, *J'*). These distortions have a dynamic origin and have been attributed to the atomic μ_3-O vibration without invoking a Jahn–Teller (JT) coupling to account for the lifting of the degeneracy of the low-lying doublets.

Here, we report a combined gas-phase and periodic ab initio study of μ_3-oxo-bridged Fe_3 triangle $[Fe_3(\mu_3\text{-}O)(CH_2FCOO)_6(H_2O)_3]^+$, extracting isotropic exchange and Dzyaloshinskii–Moriya (DM) coupling constants from DFT and post-HF calculations. We show that ΔJ originates from dynamic JT coupling to ligand-centered *E* modes, while the μ_3-oxygen plays the decisive role in enabling exchange interactions. The calculated couplings agree with single-crystal magnetometry and EPR measurements, providing a unified microscopic picture of anisotropy and symmetry breaking. These insights are propedeutic for exploiting frustrated spin triangles as model platforms in spin–electric effect studies, where vibronic coupling and spin–orbit interactions mediate electric-field control of magnetism.

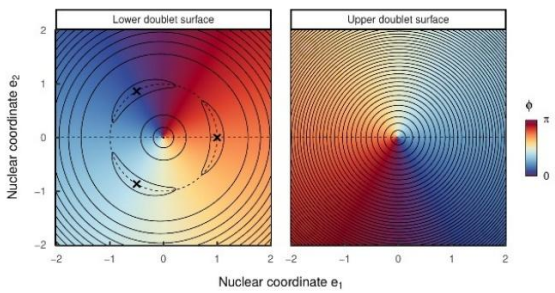


Figure 1 Contour plot of the lower (left) and upper (right) doublet surfaces in the hyper-plane spanned by the symmetry-breaking JT distortion coordinates e_1 and e_2

Computational Advancement towards Efficient Energy Materials: Connecting a Few Dots

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ABSTRACT: In this talk, I would like to present a **three-fold** research activity interconnected with a common string "**Energy**". I will start with the brief introduction of electronic structure calculations based on density functional theory (DFT) formalism, and how it could be connected to the computational screening for achieving highly efficient energy materials. The first part would be dedicated to the fundamental mechanism for the solar irradiated water splitting in *photocatalytic materials* with the future prospect of Non-linear Poisson Boltzmann Solver development for the heterogenous catalytic mechanism. The relevant exploration of novel 2D materials and their applications in such catalytic mechanism would be elaborated subsequently. The mechanism corresponding to Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER) under the influence of doping and vacancy defect from DFT based theoretical perspective would be discussed along with our recent high throughput computational investigation of finding efficient HER catalytic materials based on transition metal tri-chalcogenides. The next part of the talk would be devoted to the fundamentals and possible implications of Rashba phenomena in non-centrosymmetric structural materials and how it could govern the enhancement of catalytic efficiency, with an example case-study of BiClS janus monolayer for HER activity. We have recently successfully demonstrated the effect of strain on the overpotential of the novel catalytic materials through the tuning of Rashba splitting under the influence of external strain. I will end my talk with our recent successful endeavour of pre-intercalation mechanism in Li-ion battery, which appeared in Nature Materials, along with a few other examples where computational advancements have been in the driving seat for new materials discovery.

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Impact of Microplastic Structure and Aging on Cefixime Adsorption Dynamics

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Microplastics (MP) are pervasive environmental contaminants that can adsorb a diverse array of pollutants.[1,2] Herein, the adsorption dynamics of cefixime (Cef) antibiotic on MP comprising single and dual polyethylene (PE) chain configurations are investigated using MD simulation methods. It is predicted that the dual PE chain model exhibits a significantly higher Cef adsorption in comparison to that of a single chain. Furthermore, aged MPs show enhanced adsorption compared to their pristine counterparts. Analysis of RMSD, RDF, and MSD from simulations confirm the stability and persistence of MP-Cef interactions. It is predicted that aging facilitates stronger binding of Cef to MP. The interaction energy of Cef with PE exhibited a substantial increase upon moving from pristine (−75 kJ/mol) to aged (−345 kJ/mol) condition, indicating that aged MP may serve as important carriers of antibiotics in the environment, potentially extending their bioavailability, thus contributing to the increased antibiotic resistance in organisms. This study underscores the influence of structural variation as well as aging of MP in regulating antibiotic adsorption dynamics.

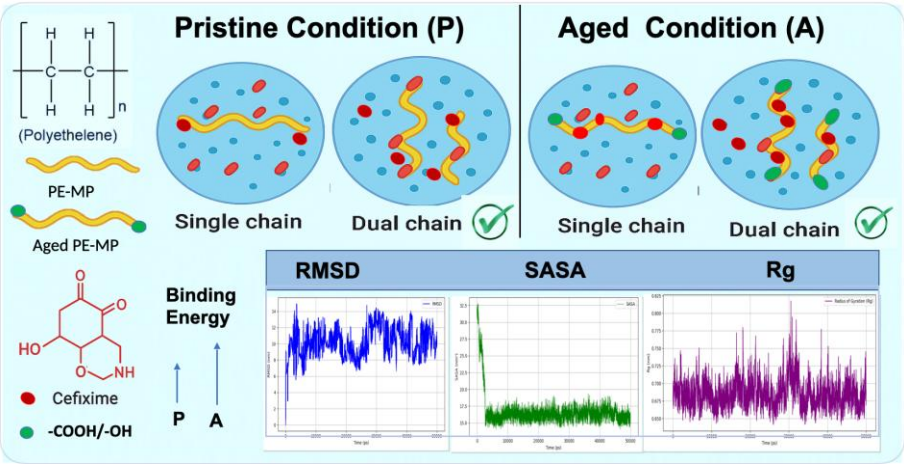


Figure 1. Schematic representation of MP-Cefixime interaction investigated in this work.

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Coupled Electronic, Structural, and Dynamical Optoelectronic Responses in Nanomaterials

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The ultrahigh surface area of two-dimensional materials can drive multimodal coupling between optical, electrical, and mechanical properties that leads to emergent dynamical responses not possible in three-dimensional systems. We observed [1] that optical excitation of the WS_2 monolayer above the exciton energy creates symmetrically patterned mechanical protrusions which can be controlled by laser intensity and wavelength. This observed photostrictive behavior is attributed to lattice expansion due to the formation of polarons, which are charge carriers dressed by lattice vibrations. Scanning Kelvin probe force microscopy measurements and density functional theory calculations reveal unconventional charge transport properties such as the spatially and optical intensity-dependent conversion in the WS_2 monolayer from apparent n- to p-type and the subsequent formation of effective p−n junctions at the boundaries between regions with different defect densities. The strong opto-electrical-mechanical coupling in the WS_2 monolayer reveals previously unexplored properties, which can lead to new applications in optically driven ultrathin microactuators.

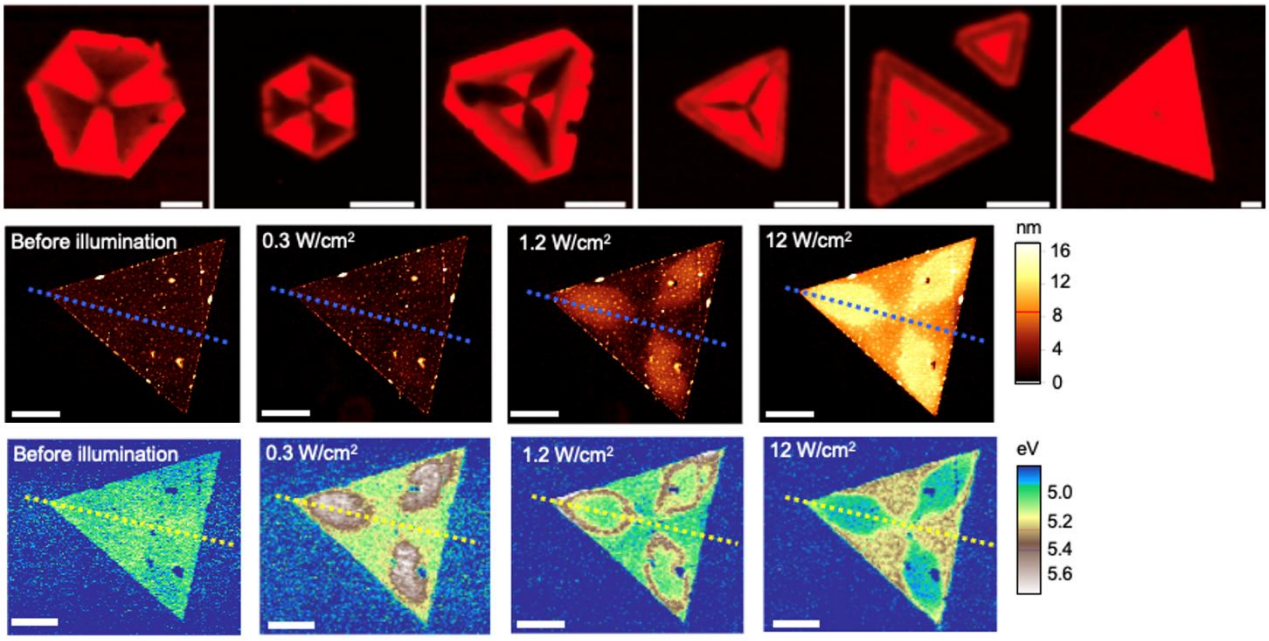


Figure 1 (top) WS_2 nanoflakes offer intricately coupled optical, mechanical, and electronic responses that vary with illumination intensity. (middle) Increasing illumination causes mechanical deformations of a triangular flake into a trefoil pattern. (bottom) A cascade of work function changes under increasing illumination highlight complex nanomaterial carrier dynamics.

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Role of protein-protein interactions in molecular mechanism of biological copper trafficking

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A key step in biological copper trafficking is the transfer of Cu(I) ion from the copper chaperone to the metal binding domain (MBD) of a Cu-ATPase residing on the membrane of an intracellular organelle. The molecular mechanism of the transfer process constitutes sequential formation of multiple covalently linked copper mediated protein-protein complexes. NMR studies and Molecular Dynamics (MD) simulations revealed existence of strong electrostatic interactions in a late-stage intermediate and highly fluctuating nature of the Cu-binding loop of apo-MBD. Because of a timescale separation between protein motions and the chemical event of bond formation, several scenarios could unfold in the early stages of the transfer process. To understand these unexplored mechanistic issues, we employed a multipronged computational approach which consists of free energy calculations, advanced analysis based on brute-force classical MD simulations and QM/MM MD simulations. Using these approaches we studied the energy landscape and association mechanism of protein-protein complexes between Cu(I)-loaded holo-chaperone and apo-MBD from yeast. This was followed by the investigation on the energetics of early stages of chemical reactions responsible for the Cu(I) transfer process. In order to get a robust understanding of the free energy landscape of such a fluctuating system, multiple methods needed to be employed. Our calculations revealed a new minimum, where proteins were arranged in a more open conformation separated by solvent, along with a tightly bound complex with multiple salt bridges resembling the experimental structure. Unbiased trajectories launched from the free energy basins, aided by QM/MM calculations, confirmed the existence of multiple reaction channels with varying degrees of inter-protein electrostatic interactions. These results suggested that the initial stages of the multi-step copper transfer were not entirely driven by electrostatic control and a significant role of protein dynamics. However, electrostatics played a crucial role. Without the minimum number of salt bridges, no ensemble with significant population was found that could lead to a productive chemical reaction. The interplay between these two effects is a manifestation of enthalpy-entropy compensation. From a functional perspective, our findings indicate that this essential biological pathway evolved to maximize the rate of transfer without optimizing the strong binding of trafficking partner proteins.

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Functionalized MOFs for Selective CO_2 Capture and Conversion

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The development of advanced materials for efficient CO_2 capture and conversion is crucial to mitigate climate change. Porous material like Metal organic frameworks (MOFs) and Zeolitic imidazolate frameworks (ZIFs), when combined with ionic liquids (ILs), promote selective CO_2 adsorption.[1-8] Employing DFT and GCMC simulations, we explored ILs impregnated MOFs and ZIFs to understand the structure property relationships influencing CO_2 affinity as well as selectivity under confinement. It is interesting to note that hydrophobic IL exhibits stronger CO_2 adsorption under confinement.[1-5] This is due to the similar hydrophobicities (*i.e. like-like pair*) of ZIF-8 framework and the selected ILs. In addition, binary mixtures of hydrophobic IL@ZIF-8 promoted CO_2 selectivity up to 3.5-fold.[3] UiO-66-based composites having aromatic cations ($[BPy]^+[BF_4]^-$) showed enhances 65% in CO_2/N_2 selectivity *via* π–π and van der Waals (vdWs) interactions, while aliphatic cations ($[N_{2224}]^+$) suffered from steric hindrance. Metal-based anions ($[AlCl_4]^-$, $[FeCl_4]^-$) further improved adsorption enthalpy and CO_2/CH_4 and CO_2/N_2 selectivity.[8] Our studies provide molecular-level insights into IL framework synergy, driving the rational design of next-generation IL@MOF materials for CO_2 capture, separation and catalytic conversion into other products.

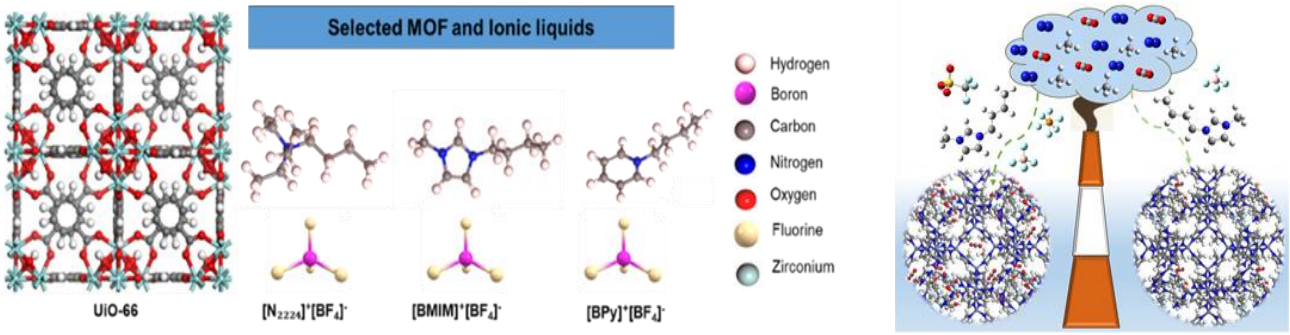


Figure 1 Representative MOF structures (i.e UiO-66 & ZIF-8), and the selected ionic liquids (ILs) used in this study, along with their pictorial application in CO_2 capture and separation.

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CHEMONTO: Leveraging Chemical Knowledge for Smarter Reaction Network Exploration

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CHEMONTO [1] is a computational framework that integrates chemical ontology with structural insights to extract knowledge from reaction intermediates during automated path searches (Figure 1). Combined with AFIR [2], it efficiently captures key intermediates and steps even in high-energy regions while filtering out irrelevant pathways to cut computational cost. Using ERPOs, reaction rules, and system setup as inputs, CHEMONTO enables broad, training free application to organometallic systems, offering a powerful tool for mechanistic studies and catalyst design.

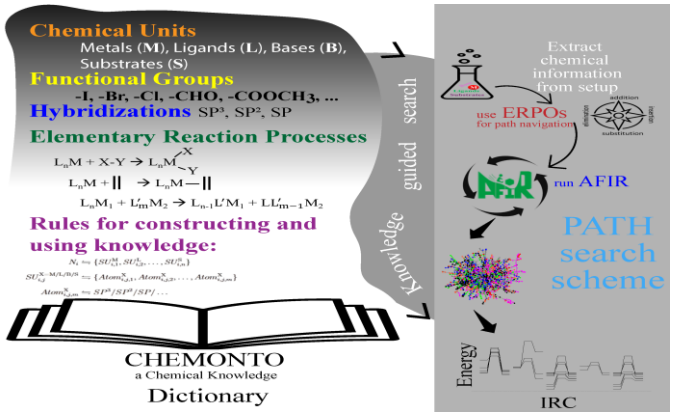


Figure 1 CHEMONTO and its working principles is shown. CHEMONTO is a knowledge dictionary. It is loaded with chemistry knowledge. It understands the concept of chemical units, functional groups, atomic hybridization, elementary reaction processes.

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Our recent attempts in computational designing of photosensitizer for photodynamic therapy application

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Photosensitizers (PSs) are the photo-acftive molecules used in various applications such as Dye-sensitized Solar-cells (DSSCs), photodynamic therapy (PDT) to mention a few. A molecule to be used as a PS for different applications needs to fulfill specific criteria. For last few years our group is focused on designing PSs for different applications in particular two-photon PDT. We use, in particular, different computational chemistry tools such as the state-of-the-art electronic structure methods *e.g.,* RI-CC2, and molecular docking and MD Simulation to study the relevant properties of different types of molecules. In this talk, I'm going to give a brief of our attempts.

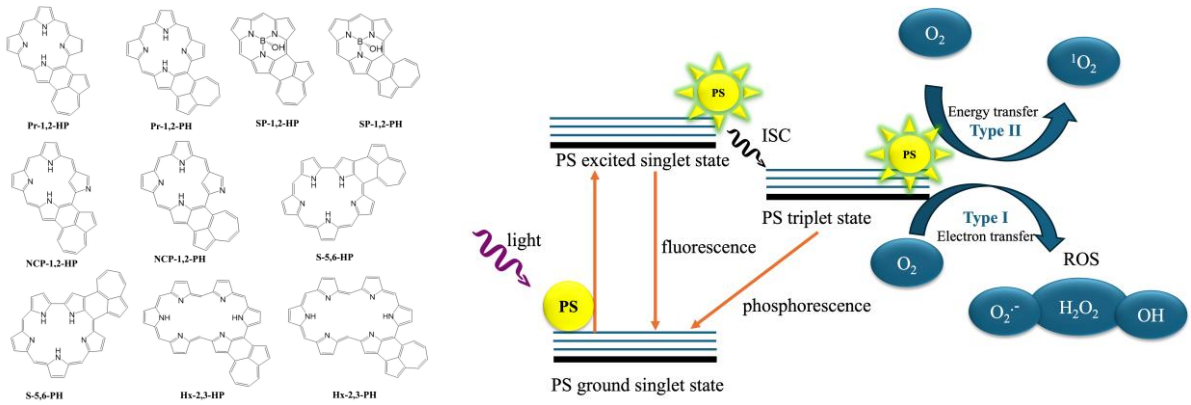


Figure 1 (Left panel) Some new molecules to be used as PSs in TP-PDT, and (Right panel) schematic of the photophysical properties involved in photodynamic therapy

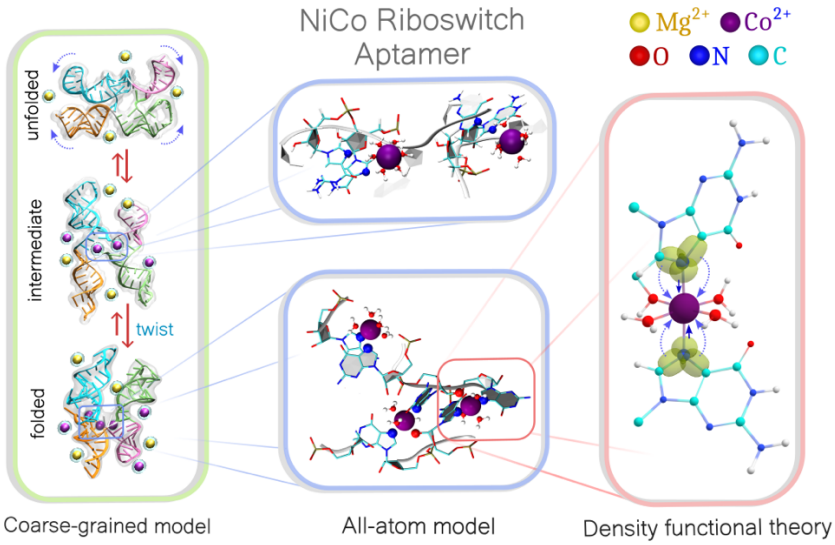
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Transition Metal Ion Sensing by Riboswitches

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Transition metal ions are crucial for bacteria survival. Bacteria employ metalloregulatory riboswitches to respond to varying metal ion concentrations. The czcD (NiCo) transcription riboswitch specifically senses Co^{2+}, Ni^{2+}, and Fe^{2+} ions at micromolar concentrations amid millimolar Mg^{2+}. We used computer simulations with multi-resolution RNA models to understand how global conformational changes in the NiCo riboswitch are coupled to the remarkable specific binding of Co^{2+}. We show that the riboswitch folds through an intermediate state, where a partially folded four-way junction (4WJ) creates an anionic pocket large enough to accommodate the binding of solvated divalent ions. The binding of Co^{2+} is coupled to the stability of the weak non-canonical G•A base pairs at the helical junction that drive the formation of native-like coaxial stacking of four helices. The Co^{2+} binding further twists the 4WJ, which locks the ions in the bound state. Electronic structure calculations show that enhanced orbital interactions between conserved guanines in the 4WJ and Co^{2+} are responsible for the high specificity of the riboswitch in binding to Co^{2+} over Mg^{2+}. We provide a framework for understanding and engineering tunable RNA-based biosensors and developing antimicrobials, as metal intoxication is an evolutionary strategy to inhibit bacterial growth.

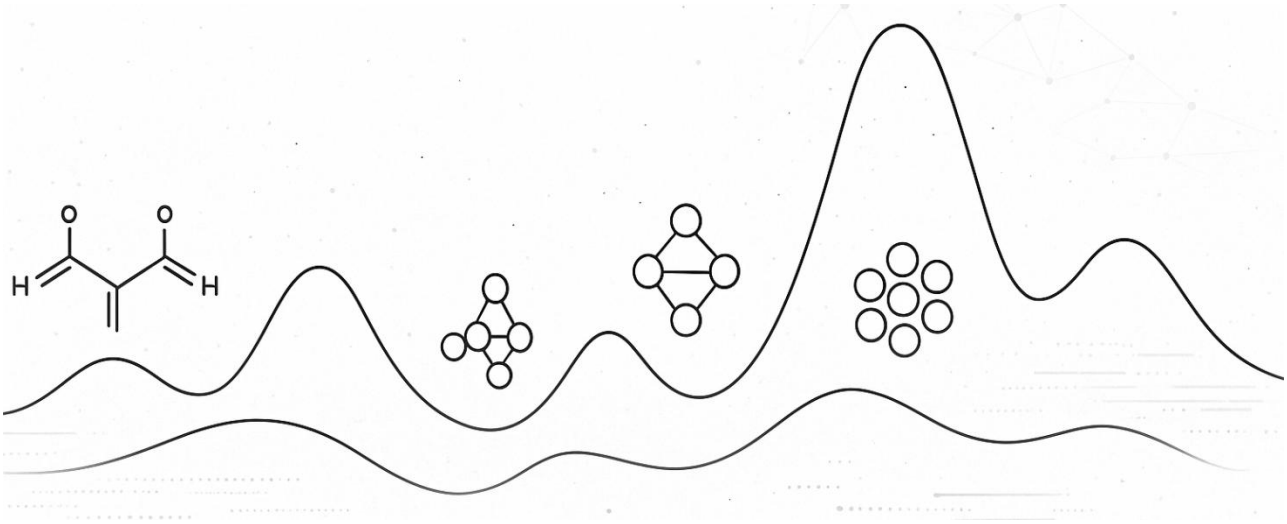


Modeling of the folding of the NiCo transcription riboswitch and its Co^{2+} ion sensing mechanism

Uncovering Structure in Chemical Space: Automated and Data-Driven Approaches

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Chemical systems, whether molecular, atomic, or larger assemblies, exist on potential energy landscapes that show how stable and structured they are. To understand these landscapes, we must look beyond finding stable points and study how shape, bonding, and interactions create overall order. In this work, automated search methods combined with machine-learning potentials are used to explore these landscapes for hydrocarbons, molecular clusters, and metal aggregates. This mix of automation and physics-based modeling helps find patterns and structures that older methods often miss. The aim is not just to locate new stable forms but to learn what these forms say about how chemical systems organise themselves — how stability emerges, how bonding spreads across atoms, and how systems move from molecules to larger materials. This study presents a view where automation is not only a tool but also a way to understand the geometry of matter.



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Q: How to Generate Unique Machine Readable Representations of Conformers, Tautomers, Transition States, Excited States, Molecular Clusters, Non-Equilibrium Geometries and Potential Energy Surfaces? An Answer: Singular Value Decomposition of Cartesian Co-ordinates (T & C Apply)

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Abstract

There exist a plethora of machine readable representations of molecules and chemical structures. They each have their own advantages and disadvantages. Even the most sophisticated method has difficulty with representing molecular conformations, incorporating stereoelectronic features, and coming up with unique representations for excited states and non-equilibrium geometries. In this work, we shall present how the singular value decomposition of the cartesian co-ordinates (w.r.t a fixed origin, and orientation) offers an excellent way to create unique machine readable representations of all the systems mentioned in the title. The implementation of this method, key illustrations, various drawbacks and its scope shall be presented herein.

Brownian Information Engines: The Essentials for Best Performance

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Understanding the interplay between thermodynamics and information of systems has become a fundamental challenge in nonequilibrium statistical physics since the emergence of the gedanken experiment of "Maxwell's demon" [1]. This demon inspects gas molecules in a single heat bath and utilizes the obtained information to extract work, thus emanating the notion of the information engine. Information engines can be considered as cyclic feedback processes that utilise information about the system's microscopic state to extract work from a single heat bath [1]. A typical Brownian information engine (BIE) consists of an overdamped Brownian particle trapped in a one-dimensional harmonic potential and connected to a single thermal reservoir. In a BIE, the feedback step is related to a sudden change in the potential energy, and hence, the information that is essential for a non-zero work output. The net (available) information, therefore, can be monitored by tuning: (a) the strength and nature of the fluctuating energy bath (often thermal) [2], (b) the shape of the confining potential (often harmonic potential) [3,4], and (c) the feedback control strategy [5]. In this talk, we will discuss the information-energy exchangeability conditions in the presence of a self-propelled environment [2], spatially varying confinements [3,4], and the control strategy of the feedback [5].

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Reduced density matrix approaches to describe photoinduced proton-coupled electron transfer

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The H/D isotope effect is the key distinguishing factor between photoinduced electron transfer (ET) and proton-coupled electron transfer (PCET) reactions. We employ density matrix approaches such as the Redfield, Coherent Modified Redfield theory and Variational Polaron to analyze the isotope effect at small to large phonon bath reorganization energies. The Variational Polaron formalism can successfully interpolate between the traditional Redfield theory at small bath reorganization energies and the full polaron transformation at large bath reorganization energies. The donor-acceptor vibronic spacing and overlaps of the nuclear wavefunctions play a key role in determining whether the isotope effect is normal or inverse. This is especially so when the bath reorganization energies are small. We also capture the vibrational relaxation of the proton mode by directly coupling the proton to the phonon bath modes. This enables us to analyze the isotope effects for the cases when the electron and proton phonon baths are uncorrelated, positively correlated or anti-correlated.

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Stochastic Resetting Prevails Over Sharp Restart for Broad Target Distributions

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Resetting has been shown to reduce the mean completion time for a stochastic process. The time between two consecutive resetting events is drawn from a waiting time distribution that defines the resetting strategy or protocol. Previously, it has been shown that deterministic resetting process with a constant time period, referred to as sharp restart, can minimize the mean time to reach a fixed target. We consider the more realistic problem of a target positioned at a random distance from the resetting site, selected from a given target distribution[1]. We introduce the notion of a conjugate target distribution to a given waiting time distribution. For this conjugate target distribution, the waiting time distribution extremizes the mean time to locate the target. In the case of diffusion we derive an explicit expression for the conjugate target distribution to a given waiting time distribuition that holds in arbitrary spatial dimension. Our results show that stochastic resetting prevails over sharp restart for target distributions (Fig 1) with exponential or heavier tails.

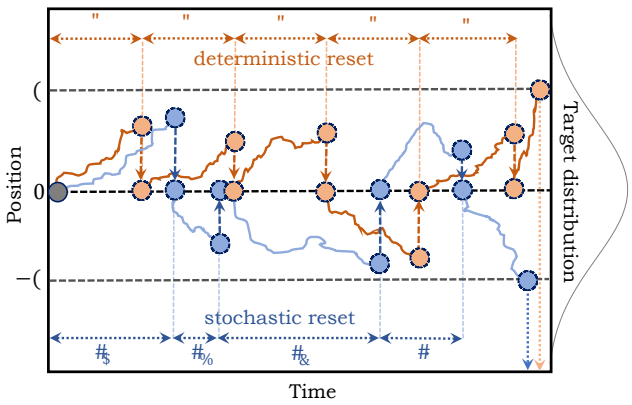


Fig 1: A schematic position vs time diagram for diffusion with resetting (in 1D). An absorbing target is located at a random distance chosen from a distribution of target centered around the origin (in gray). Two types of resetting protocols are illustrated. The red trajectory is subject to deterministic,periodic reset, i.e., where two consecutive resetting events occur after a constant interval of time. The blue trajectory is subject to stochastic reset, where the time intervals between the resetting events are taken from a waiting time distribution.

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Analytical solutions in model polymer systems

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Our one-dimensional model polymer system, constituting a flexible polymeric transducer pulled by a constant force, connects to a rigid fixed substrate by interconnecting bonds that rupture and rebind stochastically. Stochastic simulation of the model system yields a distinct steady state[1] and the associated propagating solution[2] in bead and bond dynamics. I discuss the analytical solutions to the observed phenomena, which provide insights into the relative motion between soft rubbing surfaces at the single polymer level.

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pH-Driven OprM Gating and Allosteric Control in MexAB-OprM/AcrB Efflux Pumps

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Efflux pumps are crucial transport systems that enable bacteria to expel a broad range of antibiotics, making them central to antimicrobial resistance. Understanding the underlying biophysical mechanisms is therefore essential. This study focuses on the outer membrane factor (OMF) OprM of the MexAB-OprM complex, which acts as the final conduit for drug expulsion. Using computational simulations, we investigated the pore-opening mechanism of OprM and identified metastable intermediates between its open and closed conformations. Constant pH molecular dynamics revealed that OprM exhibits distinct structural states above and below pH 5.5, confirming its pH-responsive gating behavior. Furthermore, we identified an allosteric binding pocket within the transmembrane (TM) domain of MexB. Variant 1 demonstrated the strongest affinity toward this site, showing the highest energy barrier during ligand dissociation. Eigenvector centrality analysis quantified the communication between the TM and porter domains of MexB, highlighting an allosteric network critical for efflux function. In the related AcrB pump, we observed an additional inhibitor-binding site within the TM helices, distinct from the classical distal periplasmic pocket, with inhibitors showing preference for L protomers. Three potential ligand exit pathways from the TM allosteric site were characterized. Notably, inhibitor binding disrupted inter-domain signaling, evidenced by an increased shortest path distance between Val452 and Ala831. These results underscore how inhibitor interactions modulate communication dynamics and reveal new insights into pH-dependent gating and allosteric regulation within multidrug efflux systems.

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Capturing Vibrational Excitation Patterns of Molecular Systems using Machine Learning Tools

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When a van der Waals molecule, with a large vibrational degree of freedom, is excited at high temperature, what could be the pattern of the excitation to each of the vibrational mode? In this work, we try to answer this question using a machine learning tools by analysing predissociation dynamics. Benzene dimer is chosen as a model example. In this talk, I demonstrate that one can guess (1) the dissociation dynamics of a different excitation temperature not using any data of that temperature,[1] (2) the dissociation dynamics of the molecule when all modes are randomly excited using the dissociation data of the complex when all intermolecular and intramolecular modes[2] are excited separately, and (3) the probability of excitation of different frequency modes in a simulation when all modes are randomly excited by analysing the dissociation profile.

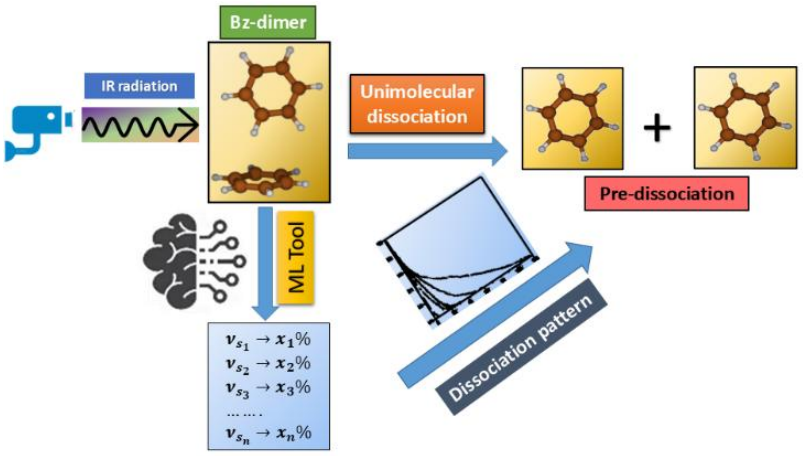


Figure 1 Schematic presentation of modus operandi

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Optimizing collective variable and enhancing protein folding transitions with explainable machine learning model: Role of hydration

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Traditionally, the choice of collective variables (CVs) in studying protein folding transitions is generally protein centric and solvent related variables are mostly ignored. Most relevant choices are fraction of native contacts, RMSD, R_G etc with particular emphasis on fraction of native contacts. Here in this study, we have chosen commonly used order parameters (OPs) (e.g: Rg, RMSD, fraction of native contacts etc.) along with solvent driven related OP to describe the folding transition. We have employed a denoising time-lagged autoencoder framework incorporating time-lagged autocorrelation functions to capture slowest variables in protein-folding which is essentially linear combinations of multiple OPs. Moreover, to construct the kinetic pathways, we have constructed markov state model (MSM). It is found that this model successfully resolved system kinetics (folding and unfolding times) quite accurately with existing experiments and identified multiple low-populated metastable basins for small proteins. Applied to chignolin mutant and Trp-cage, the method identifies misfolded conformations consistent with NMR studies. Using our developed protocol, we have characterized the contributions of different OPs near the transition state (TS). While fraction of native contacts was found to be the most important OP doe describing the global landscape, the solvent related OP is found to contribute significantly in the TS region which indicates crucial role of solvent in driving folding transitions. Next, we have derived the TS-derived CV for these systems and run enhanced sampling simulations with this CV in the framework of well-tempred metadynamics. We will discuss our preliminary results on the sampling aspects of protein folding transition using our TS-derived CV.

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Equation of motion coupled cluster with singles, doubles and full triples: Some pilot applications

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Equation-of-motion (EOM) coupled-cluster (CC) with singles and doubles (SD) is one of the most commonly used methods for accurate electronic structure computation of near-degenerate electronic states arising by excitation, attachment or detachment of electron(s). Inclusion of full triples results in the high-end EOM-CCSDT[1] method which significantly enhances the accuracy in energies and energy-gaps. We present some pilot applications of our EOM-CCSDT implementation within Q-CHEM[2] software. We also present some cost-cutting techniques that can extend the applicability of EOM-CCSDT to molecules of bigger computational size.

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Computational Insights into Boron-Catalyzed Small-Molecule Activation: From Methane Oxidation to CO_2 Utilization

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In this talk, I will present our group's recent computational investigations on boron-based catalytic reactions for the activation of small molecules such as CH_4[1,2,3,4] and CO_2[5,6]. Recent experimental studies have shown that B_2O_3 and boron nitride catalysts, in the presence of O_2, can activate methane to form formaldehyde. Boron nitride has also demonstrated the selective oxidation of light alkanes (ethane, propane, and butane) to alkenes, while B_2O_3 catalyzes the cycloaddition of CO_2 with epoxides to yield cyclic carbonates. Additionally, BPh_3 has been reported to catalyze CO_2-epoxide coupling reactions.

Motivated by these advances, our group has carried out detailed DFT-based mechanistic studies to unravel the reactivity of boron-based catalysts. For B_2O_3-catalyzed methane-to-formaldehyde conversion, we considered both crystalline and molten B_2O_3, given that the reaction occurs at ~823 K, above the melting point of B_2O_3 (~725 K). Using a range of possible active sites, we found that in the molten phase, B−B sites are more favorable than the usually known B−O−B sites. Furthermore, both singlet and triplet O_2 were investigated to account for high-temperature conditions. Our results reveal that O_2 activation enables the conversion of CH_4 to HCHO, with CO observed as a side product, while CO_2 formation is kinetically unfavorable, consistent with experimental findings.

In the later part of the talk, I will present our DFT results on boron nitride catalysis for methane oxidation in the presence of O_2, followed by our mechanistic insights into boron-catalyzed CO_2-epoxide coupling leading to cyclic carbonates. Together, these studies provide fundamental insights into the role of boron-based catalysts in small-molecule activation and sustainable transformations. Finally, I will also show our recent DFT results on the reactivity of copper-based catalysts to activate methane and other similar C−H bonds.[7,8]

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Lipid Vesicle Behavior in Ethanolic Environment: Swelling, Rupturing, Aggregation, and Fusion

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Ethanol is known to enhance lipid membrane permeability and induce significant structural changes in the morphology and aggregation behavior of lipid vesicles.[1,2] We will present our recently published work,[3,4] where we fdeveloped an ethanol model and employed coarse-grained molecular dynamics (CG-MD) simulations involving millions of particles to investigate vesicle aggregation and fusion in presence of ethanol. Our results show that the size of a biomimmetic and bacterial lipid vesicles increases with ethanol addition, reaching a maximum at 30 mol%.[3,4] We also observe vesicle swelling and a reduction in bilayer thickness as ethanol concentration rises to 30 mol%. Beyond this threshold, vesicles lose structural integrity and begin to rupture. Fusion studies reveal that vesicles can successfully fuse at ethanol concentrations between 20 and 30 mol%, provided they are brought within a critical distance at the appropriate concentration. Furthermore, multi-vesicle simulations indicate that vesicle enlargement enhances aggregation likelihood at higher ethanol concentrations.[3] Finally, we will discuss how cholesterol mitigates ethanol-induced destabilization of vesicles.[5]

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Computational Studies to Explore Metal Organic Framework Materials for CO_2 Capture from Flue Gas Mixture

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Metal organic frameworks (MOFs) are the ordered inorganic-organic hybrid porous materials with potential applications in separation and storage of different important gases like H_2, CO_2, CH_4 etc.[1-2] Advanced computational techniques like computational high-throughput screening (HTS) and machine learning models are shown to be powerful tools to screen a large database of materials and identify the top performing candidates for specific application.[3-4] Through computational HTS studies using a multi-scale modeling strategy, we tried to identify the top MOFs for CO_2 capture and understand the nature of confinement and chemistry responsible for efficient CO_2 capture from flue gas mixture. We also tried to functionalize the ligand with complementary organic motifs with precise charge alignment complementary to CO_2 atomic charges to enhance the CO_2 adsorption energy in MOFs. To accelerate the HTS studies further, we attempted to train, test and validate a machine learning model that can predict the CO_2 loading capacity in MOFs from a CO_2/N_2 binary mixture. For this study, publicly available dataset, the Quantum MOF (QMOF) database consisting of around 20,000 MOF structures is considered. For all the MOFs, different pore structure related properties like pore limiting diameter (PLD), largest cavity diameter (LCD), accessible volume (AV) and accessible surface area (ASA) are measured. From the database, MOFs with PLD greater than the kinetic diameter of CO_2 molecule are only considered to simulate the adsorption properties. Adsorption of CO_2/N_2 mixture at 1 bar pressure and 313 K has been simulated using the grand canonical Monte Carlo (GCMC) simulations to measure the CO_2 loading capacity and CO_2/N_2 selectivity. Feature space that can represent both the physical and chemical nature of the pores in MOFs has been considered for training the model includes. Different regression algorithms were considered to train the model and decision tree based model has been shown to give better predictions. Hyper-parameter tuning has been considered to further improve the model predictability.

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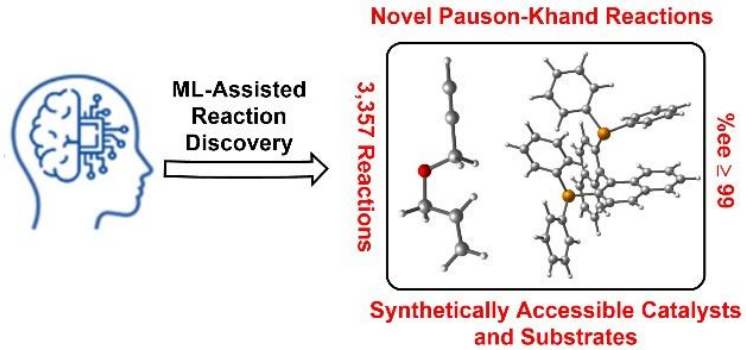
Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

AI-Driven Discovery of Asymmetric Pauson-Khand Reactions: A New Toolbox in a Synthetic Chemist's Treasure

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Asymmetric Pauson-Khand reaction is widely used for synthesis of enantiopure five-membered cyclopentenone which is an essential building block for construction of complex molecular architectures with high stereochemical precision.[1] However, the enantiomeric excess (%ee) obtained in this reaction is significantly impacted by both the structural complexity of substrates and catalysts and the reaction conditions like temperature, solvent polarity, and CO gas pressure.[2,3] A direct correlation between the reaction output (%ee) and the molecular/non-molecular descriptors is still unknown even in today's date which is a significant challenge for judicious reaction design. In the present study, we have used a robust machine learning model and discovered a library of 3,357 new Pauson-Khand reactions by engaging experimentally unknown combinations of the catalysts, substrates, and reaction conditions. These new reactions have been predicted to have %ee ≥99. Four different machine learning algorithms have been used: extreme gradient boosting, random forest, light gradient boosting machine, and neural network. The axially chiral biaryl catalysts and 1,6-enyne substrates, present in our library, is synthetically accessible.



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Modelling of Excited State Properties in Narrow-Band Organic Emitters

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Abstract:
In my talk, I will present our work on excited-state radiative and non-radiative processes in narrow-band organic emitters. First, I will introduce the different types of narrow-band emitters. Then, I will present our recent works on multi-resonant thermally activated delayed fluorescence (MR-TADF) molecules, a class of narrow-band organic emitters that are increasingly being explored for their applications in optoelectronics and display technologies. However, accurately modelling their singlet–triplet energy gap (ΔE_{ST}) remains a significant computational challenge due to the short-range charge-transfer (SRCT) nature of their excited states. I will describe in detail the methodology we have developed to calculate the excited-state properties of MR-TADF molecules.

Keywords: Narrow-band, TADF, Excited State, OLED

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Computational prediction of new molecular candidates for delayed fluoroscence from inverted singlet and triplet states

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Thermally activated delayed fluorescence (TADF) enables 100% exciton harvesting in organic light-emitting diodes (OLEDs) through an endothermic reverse intersystem crossing (RISC) when the S1-T1 energy gap is small. A new mechanism that has been found in triangular molecules with a nitrogen core involves delayed fluorescence from an inverted (i.e., negative) singlet-triplet gap (DFIST)[1]. We have generated a database of excited state energies of about 13,000 small molecules and found there is no example in the small molecule chemical space exhibiting this unusual negative S1-T1 gap, which violates Hund's rule[2]. We have also found that molecules in their high-symmetric structures showing negative gaps cease to exhibit this behaviour when distorting to more stable, low-symmetric structures[3]. Heteoatom-substituted polycyclic aromatic hydrocarbons have shown the potential for identifying DFIST candidates in various structural forms, ranging from planar to helical, opening up the possibilities for developing next-generation light emitters[4].

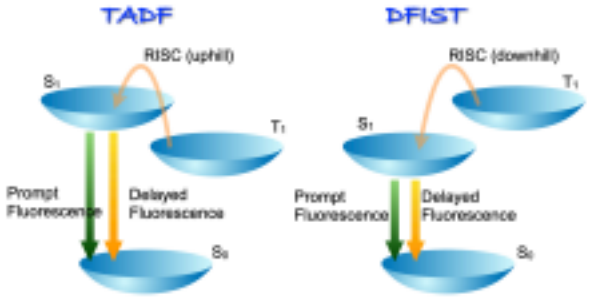


Figure 1: Potential energy surface characteristics of TADF and DFIST emitters

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Resolving Density-Driven Errors in Kohn—Sham and Post Kohn—Sham Methods: From Molecules to Materials

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Kohn—Sham (KS) density functional approximations (DFAs) often present puzzling errors in the form of overbinding for weak-intermolecular interactions and surface-adsorption problems. On the other hand, post-KS DFAs, such as the random phase approximation (RPA), often show underbinding for similar problems. Here we show that the root cause for such errors is density-driven rather than the quality of the exchange-correlation approximation. For KS methods, the errors can be remarkably minimized by using Hartree-Fock density,[1] while for the case of post-KS RPA, we propose self-consistent and perturbative singles corrections.[2] The power of these methods is demonstrated across a variety of systems, including dimers of closed- and open-shell molecules, and for molecular adsorption on ionic materials.[3]

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Buckets Instead of Umbrellas for Enhanced Sampling and Free Energy Calculations

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Umbrella sampling has been a workhorse for free energy calculations in molecular simulations for several decades. In conventional umbrella sampling, restraining bias potentials are strategically applied along one or several collective variables. Major drawbacks associated with this method are the requirement of a large number of bias windows and the poor sampling of the transverse coordinates. In my presentation, I will introduce an alternate formalism that departs from the traditional umbrella sampling to mitigate these issues, where we replace umbrella-type restraining bias potentials with bucket-type wall potentials. This modification permits one to formulate an efficient computational strategy leveraging wall potentials and metadynamics sampling. This new method, called “bucket sampling”, can significantly reduce the computational cost of obtaining converged high-dimensional free energy surfaces. Extensions of the proposed method with temperature acceleration and replica exchange solute tempering will also be demonstrated.

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Using Deep Learning models to predict mixed quantum-classical trajectories

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Deep learning models are increasingly being integrated into mixed quantum–classical trajectory simulations to accelerate the evaluation of potential energy surfaces and nonadiabatic couplings. By learning high-fidelity quantum-mechanical information from training data, these models can replace or augment expensive ab initio calculations during dynamical propagation. This synergy enables large-scale, long-timescale simulations of photochemical and reactive processes that were previously computationally prohibitive with traditional quantum-chemical methods alone. The last few years has seen a great deal of thrust in this area. Our group recently started exploring this as well, and we present our findings in this regard by first exploring non-ML time-series model-fitting results, and how badly they perform, and then delve into deep-learning based models and evaluate their performance in predicting the potential energy surface as a first step. As the next step we will be looking to collaborate with groups that work on improving the accuracy of the electronic inputs that go into these models both in ground and excited state dynamics.

Insights into the Molecular Mechanisms in Biology using Modeling and MD Simulations

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Proteins, being the polymers of α-amino acids, have incredible number of accessible conformations. But for each protein, only a small region of that vast conformational space is relevant for function, which is known as native state and it is also likely to be the most populated region in principle. Molecular Dynamics (MD) simulation-based sampling methods, and focused around ensemble of conformations in the vicinity of the native state has been proven to be useful to provide mechanistic insights into the processes in biology. While the statistical significance of the sampling timescale is important to claim the results to be realistic, in practical sense the timescales of the biological processes are still several fold higher than that the state of art computers can access. Nevertheless, strategic applications of such methods, could be useful to address questions which have much relevance in biology, e.g. obtaining insights into combating cell proliferation or even finding suitable inhibitors for a flexible receptor to combat a disease. This presentation will show, that strategic applications of modelling and simulations can really help address questions in Biological sciences of practical importance, which are otherwise difficult to answer form state of art experiments and can really take the scientific understanding forward. This presentation will show some examples of applications made in recent time, e.g. tubulin-microtubule[1] dynamics in the context of cell proliferation, kinases[2] and its activation, and even ligand design etc. Our recent success on applications of machine learning based methods to identify the allosteric[3-4] communication channels and the capacity to take context dependent judgement will also be discussed.

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Integrating Multiple Electronic Pathways in Single Molecule Breadboard Junctions

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The field of molecular electronics aims to develop functional circuits comprised of molecular components. To further this vision, we have introduced the concept of electronic molecular breadboards as a framework to study and prototype circuit combinations within the Scanning Tunneling Microscopy (STM-) or Mechanically Controllable break-junction (MC-BJ) setup [1]. I will discuss the development of new computational models to simulate conductance histograms from STM-BJ/MC-BJ experiments of molecular breadboard junctions[2,3]. I will also show how such models can allow researchers to experimentally access the embedded circuits within the molecular breadboards[3].

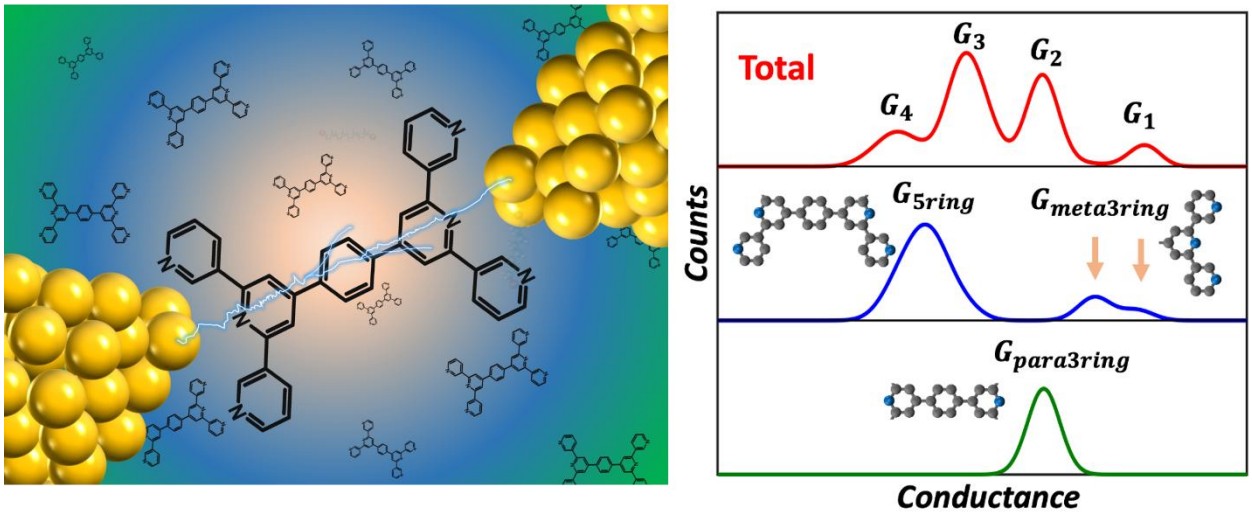


Figure 1 Molecular Breadboards Junctions such as the 6-terminal Bis-terpyridine system (Right panel) have conductance readouts originating from multiple embedded circuits. Our models enable us to deconvolute these complex readouts (Left panel) and access/tune the electronic response of the embedded circuits.

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Towards the binding of S-Peptide to S-Protein in the S-Peptide S-Protein Complex (RNase S)

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The folded conformation of a protein is crucial for its enzymatic function as it establishes the structural framework necessary for substrate identification, active site arrangement, stability, conformational changes, catalytic mechanism, and control. Ribonucleases, also known as RNases, have essential functions in biological systems as they facilitate the breakdown of RNA molecules into smaller fragments by catalysis. RNase S is a heterodimeric protein consisting of two units: S-Peptide (S1) and S-Protein (S2). The S-Peptide acts as the catalytic component, responsible for the ribonuclease activity of the enzyme. S-Protein subunit plays a structural function by maintaining the overall shape of the enzyme. Precise folding of the biomolecule is essential for the formation of the active site, promoting the identification and attachment of substrates, preserving stability and flexibility, and enabling the catalytic process. Thus here we present [2] the folding-unfolding dynamics of the isolated S-Peptide and S-Peptide in the RNase S complex. Our findings confirm that the isolated S-Peptide exhibits high levels of dynamism and instability.

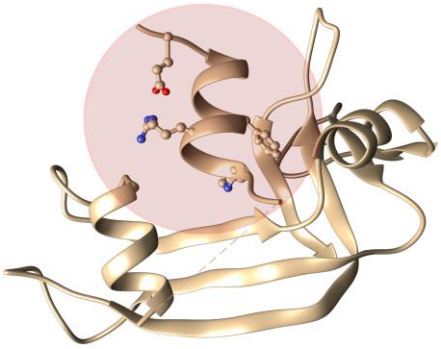


Figure 1 . Schematic representation of the RNase-S complex structure showcasing the S-Peptide (residues 1-20, the encircled one) and the S-Protein (residues 21-124).

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Theoretical Chemistry Symposium
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Preparation and coherent manipulation of toroidal moments in molecules

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Molecules with an odd number of electrons are normally expected to display paramagnetic behaviour in a uniform magnetic field. Instead, a vanishing magnetization is often measured in a special family of lanthanide complexes known as Single Molecule Toroics.[1-5] The anomaly can be explained in terms of degenerate quantum states in which electron spins and orbital currents give rise to time-odd and space-odd magnetic vortices known as toroidal moments, carrying a vanishing magnetic dipole.[6,7] Resilient to stray magnetic fields and susceptible to electric manipulation, macroscopic toroidal states are sparking growing interest for applications in spintronics, magnonics and photonics.[7-9] While macroscopic toroidal configurations have been observed in bulk condensed matter, e.g. in low-dimensional non-collinear ferromagnets,[7,9] theoretically predicted quantum toroidal states in molecules are yet to be observed, as it is currently unclear how to split degenerate states carrying counter-rotating magnetic vortices via existing experimental setups. Here we present a realistic experimental protocol to polarize and observe molecular toroidal moments using pulsed microwave (MW) radiation.[10] Modelling the spin-dynamics in a pulsed MW-field, [10,11] we find that three resonant MW-pulses, delivered either sequentially or simultaneously, to a class of MDy_6 heteronuclear complexes ($M = Al^{3+}$, Cr^{3+}) consisting of coupled Dy3 toroidal moieties, [12,13] can selectively and coherently transfer population to a long-lived polarized toroidal state.[10,14] The ensuing magneto-electric effect can then be used as a read-out mechanism,[7] thus configuring a first strategy to measure and coherently manipulate toroidal states in molecular systems.

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Enhanced Sampling and Estimation of Rare Event Kinetics in Molecular Simulation: Some Ideas and Benchmarks

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Abstract

Understanding the molecular mechanism of any complex biophysical or chemical processes requires tracking of the dynamics on the underlying (free) energy landscape. For all practical purposes, this requires projection from a higher-dimensional landscape (*3N* for *N* particle system) onto a few “collective variables” or order parameters or reaction coordinates. The accuracy of the computed free energy landscape and barrier often strongly depends on this choice of collective variables to project on. Moreover, estimation of rare event kinetics (rate constant) from the underlying free energy landscape suffers from the lack of any exact rate theory. In this talk, we shall discuss the “weighted ensemble” (WE) class of path sampling method for directly estimating rate constants of rare events without any biasing forces or elevated temperature and without pre-computing the underlying free energy barrier. We shall introduce a few variants of WE-based methods developed in our group.

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Modelling Excited States : Insights from Selected Examples

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Understanding how molecules behave in their excited states is key to explaining many chemical and physical processes - from light absorption and emission to charge transfer and reactivity. Photochemistry is now being used for cancer therapy as well ! Yet, accurately modelling these states continues to be one of the most demanding tasks in molecular quantum chemistry. Excited states come in many forms - localized valence excitations, diffuse Rydberg states, charge-transfer transitions, or open-shell configurations - and each poses unique challenges for theory and computation.

This talk explores a set of illustrative molecular examples to show how different theoretical methods capture these diverse types of excitations. We will compare widely used single-reference approaches such as time-dependent density functional theory (TDDFT), configuration interaction singles (CIS), EOM-CC, etc. with more sophisticated multi-reference methods like CASSCF, various MRPT2, MRCI and MRCCs. The discussion will highlight common difficulties such as spin contamination, state mixing, and the correct treatment of double and near-degenerate excitations - issues that often determine whether a calculation gives the right picture or not.

By walking through these examples, the presentation will emphasize how choices like the active space, basis set, or functional affect the quality of results, and when a simple method can be trusted versus when a more elaborate one is necessary. While comparisons with experimental data will be mentioned briefly, the focus will be on developing an intuitive understanding of what each method can (and cannot) tell us. The goal is to provide a clear, practical view of how modern electronic structure theories tackle excited states, and how theoretical insight can deepen our understanding of molecular photophysics and spectroscopy.

Bond Breaking, Bond Making, Activating, Catalyzing: Low-Energy Free Electrons as Tunable Reagents

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Low-energy electrons (LEEs) are the smallest, most fundamental, and inherently green reagents in chemistry. Harnessing their reactivity below the ionization threshold opens a transformative frontier—one where the **controlled use of LEEs** enables **precise, tunable, and highly selective** reactivity, driving **state-, site-, and even bond-specific** chemical transformations, catalysis, and activation. At the heart of this emerging paradigm lies the **tunability of resonant interactions** between LEEs and valence electrons—the very electrons that govern molecular structure and reactivity. In this talk, I will present our recent findings that demonstrate the remarkable versatility of **resonant-interaction–driven LEE chemistry**, highlighting its role in **σ-bond selectivity**, **CO_2 activation**, and the elusive phenomenon of **free-electron hydration [1,2]**.

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Quantum Dynamics Studies of Charge-Transfer Processes in Ion-Molecule Collisions at High (keV) Collision Energies relevant to Cometary Environments

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The importance of ion-molecule collisions is well realized in Earth's upper atmosphere, cometary, and interstellar spaces. The CT processes, H^+ (He^+) + CO (N_2, O_2) → H (He) + CO^+ (N_2^+, O_2^+), are often observed in high-energy collisions that typically occur in the cometary and Earth's atmospheres, particularly during solar flares.

Our study, conducted using the MRCI/aug-cc-pVQZ level of theory, involved an extensive *ab initio* analysis of the lowest nine electronic states for the He^+ + CO (N_2) → He + CO^+ (N_2^+) systems. These investigations aim to identify and explore the potential energy surfaces and the nonadiabatic interactions involved in the charge transfer process. We have computed the non-adiabatic couplings and the quasi-diabatic surfaces using the *ab initio* procedure. The calculated strengths of the non-adiabatic couplings help identify the probable and dominant charge transfer channels, corroborating the experimental observations. 1,2

We also investigated the collision dynamics of H^+ with O_2 at high collision energies (0.096–4.848 keV) in the time-dependent semiclassical framework[3]. We have calculated dynamical attributes, such as differential and integral cross sections, for the electronically elastic and CT processes using the computed quasidiabatic surfaces and potential couplings, and compared them with available data from scattering experiments, providing a robust validation and understanding.

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Etching Silicon Oxide – Catalysis and Selectvity

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The continued scaling of semiconductor devices requires sub-nanometer precision and high material selectivity in etching to define nanoscale features in silicon-based dielectrics. Silicon oxide and silicon nitride are ubiquitous in advanced device architectures including MOSFETs, FinFETs, GAA transistors, and 3D NAND where they often coexist in stacked configurations. Selective oxide removal in the presence of nitride is critical for pattern transfer and spacer formation, demanding high oxide-to-nitride etch selectivity to preserve dimensional fidelity and dielectric integrity. Etch chemistry controls etch rate (ER), selectivity, and surface morphology through radical generation, adsorption, surface reaction kinetics, and byproduct desorption. While HF remains the conventional etchant for silicon oxide, further optimization of etch chemistries is essential to improve precision and selectivity. In this work, we employ alcohols and carboxylic acids as protic catalysts to enhance the selective etching of silicon oxide over silicon nitride. This presentation will discuss the role of protic catalysts in achieving highly selective silicon dioxide etching, highlight molecular-level interactions of catalytic species with surfaces to enable atomic layer etching (ALE) process, and examine the multilayer diffusion of neutral molecules on the sidewalls in the aspect ratio dependent etching (ARDE) under cryogenic conditions.

Quantum Computing for Computational Chemistry

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Simulating quantum systems was the foundational motivation for building quantum computers and is also a practically relevant challenge. Quantum computers have recently become competitive with the best approximate classical algorithms for quantum simulation-like tasks, and is currently approaching the accuracy of the density matrix renormalization group for electronic structure calculations. Algorithmic performance before the era of quantum error correction is a key consideration, and recent success has been motivated by (classical) computational chemistry techniques. These new sample-based methods require a hybrid computational model in which quantum computers interact tightly with classical high-performance computing[1]. Inspired by the Hubbard Hamiltonian, the local unitary cluster Jastrow ansatz is single-reference while modeling correlations in a predictably improvable manner, and is amenable to implementation on current limited-connectivity quantum hardware[2]. This interplay of classical and quantum algorithms provides evidence for near-term quantum advantage for computational chemistry.

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Role of Electric Fields in Modulating Structure-Function Relations

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Electric fields (EFs) have emerged as a powerful external stimuli which impacts geometry, bonding, reactivity, and stereoselectivity. In general, being a vector, EF catalyses the reaction in one direction while inhibiting it in the opposite direction. However, a distinct two-way catalytic mechanism of EF has been demonstrated in cycloaddition and oxidative addition reactions. The inhibition by an EF is limited for such reactions and the highest inhibitive EF is termed as electrostatic resistance point (ERP). Thus, at the ERP an inhibitive EF turns to catalytic in nature. In a Diels-Alder reaction, the ERP value marks the change in reaction mechanism between normal electron demanding and inverse electron demanding (NED vs IED) pathways. The ERP of a reaction depends on the electronic structure identity of functional groups and its orientation with respect to the EF which help to relate ERP with stereoselectivity. Two-way catalysis of EF alters the function of a Lewis acid (LA) in Oxa-Diels alder reaction and change its to a Lewis base. Two possible electron transfer pathways in opposite direction during oxidative addition either through metal-toligand charge transfer (MLCT) or ligand-to-metal charge transfer (LMCT) bring two-way EF catalysis in such reactions. The oxidative addition of aryl bromides to Pd in Suzuki-Miyaura coupling as a model reaction is further used relate EF catalysis to fundamental properties that affect a reaction such as inductive effect, electroinductive effect, and differential solvation effects. The analogue effects of EF on the reaction with these properties have been utilized to generate a unified Electric Field Equivalent (EFEq) value for substituents and solvents. The conceptual coherence derived based the EFEq, an additive quantity, is envisioned to act as a basic building block to connect the electronic effect of substituents and differential solvation with emerging EF catalysis

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Chirality Without Chiral Sources: Computational Insights

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In this talk, I will present the first computational study on the induction of three contiguous chiral centers in azabicyclic scaffolds catalysed by the frustrated Lewis acid pair (FLP).1 The selection of the FLP and an inverse hydride shuttle pathway is crucial for the transformation of achiral substrates into chiral azabicyclic scaffolds without any assistance from chiral sources.2 The strength of electron-withdrawing groups on olefins controls the need for promoters.3 To gain a deeper understanding of the key factors involved in all interesting events observed by the experimentalist, a condensed Fukui function analysis, ASM, and a detailed mechanistic study of this complex reaction were performed (Figure 1).

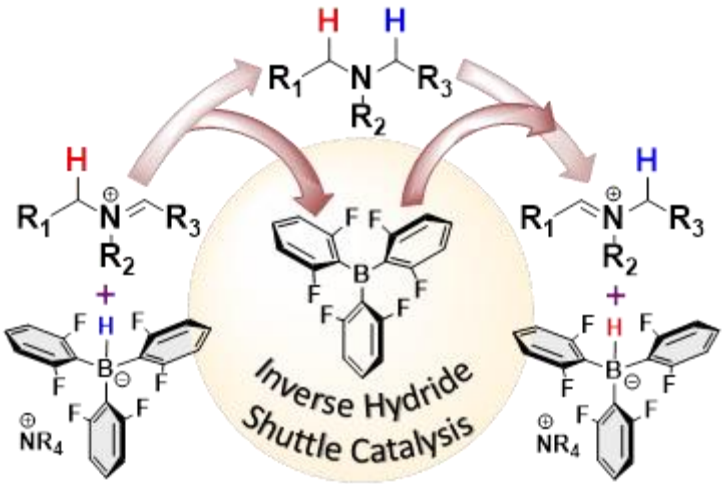


Figure 1: Inverse hydride shuttle catalysis

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AMAT

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Advanced materials science thought leader and prolific innovator with over 40 U.S. patents and 20+ international patents. Ex-GE (20 years) and Applied Materials (5 years) and is Adjunct faculty with the Department of Metallurgical & Materials Engineering, IIT Madras since April 2024. Recognized for deep expertise in materials, processing, and additive technologies, with a proven track record of delivering breakthrough solutions from lab scale to full-scale manufacturing. Contributions span a diverse suite of materials, including phosphors, scintillators, structural ceramics, coatings (TBCs & EBCs), advanced processing, and manufacturing technologies.

An **innovation coach and mentor**, enabling teams to think beyond conventional boundaries and generate differentiating intellectual property across domains. Known as an **inclusive and empowering leader**, adept at building and nurturing high-performing teams. Current interests include additive manufacturing, additive analytics, and advanced material design, with a strong focus on advancing the state of the art through collaborations with academia in India and globally on programs of industrial significance.

With over three decades of corporate research experience, I have established new research capabilities, built laboratories, and nurtured talent growth across diverse domains. Since 2017, I have been a passionate champion of industry–academia partnerships, driving innovation ecosystems that connect fundamental research with industrial application.

Certified as a **Six Sigma Black Belt** and **Associate Value Specialist (SAVE International)**, I bring rigor and value-focused methodologies to every initiative.

Having recently transitioned from corporate life, I now serve as an **Adjunct Faculty**, working closely with students and faculty to advance the frontiers of materials science and allied technologies. My current focus is on fostering collaboration, mentoring future innovators, and pushing the boundaries of advanced materials research.

Wiley

ParthaPratimPal

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Unravelling Atmospheric Reaction Mechanisms at Seawater: Insights from Ab-Initio Molecular Dynamics Study

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Atmospheric chemistry is significantly influenced by the processes occurring at the seawater. Among these, reactions between halide anions (X^-) present in the water with incoming gas-phase molecules such as hypohalous acid are of major atmospheric interest due to their role in tropospheric oxidation cycle. However, inherent complexity and multi-step nature of these reactions left their mechanisms largely unexplored. Here, we focus on the reactions between hypochlorous acid (HOCl) with anions at seawater in both interfacial and bulk aqueous environmentsusing Ab-Initio Molecular Dynamics (AIMD) simulations. The main findings are:

1) We unravel the detailed atomistic mechanism of halogen exchange reaction, $HOCl+I^- \rightarrow HOI+Cl^-$, which proceeds via a Grotthuss-like hydroxide transport involving multiple water molecules at neutral pH-a stark contrast to the gas-phase mechanism[1].

2) Whereas in acidic pH condition we observe dihalogen formation[2].

3) Intriguingly, we demonstrate the halogen bonded complexes of $[(HOCl)...(X^-)]_{aq}$ act as the reaction precursors while the hydrogen bonded complexes remain unreactive. Our studies suggest that AIMD is a powerful tool to investigate these interfacial charge transfer reactions.

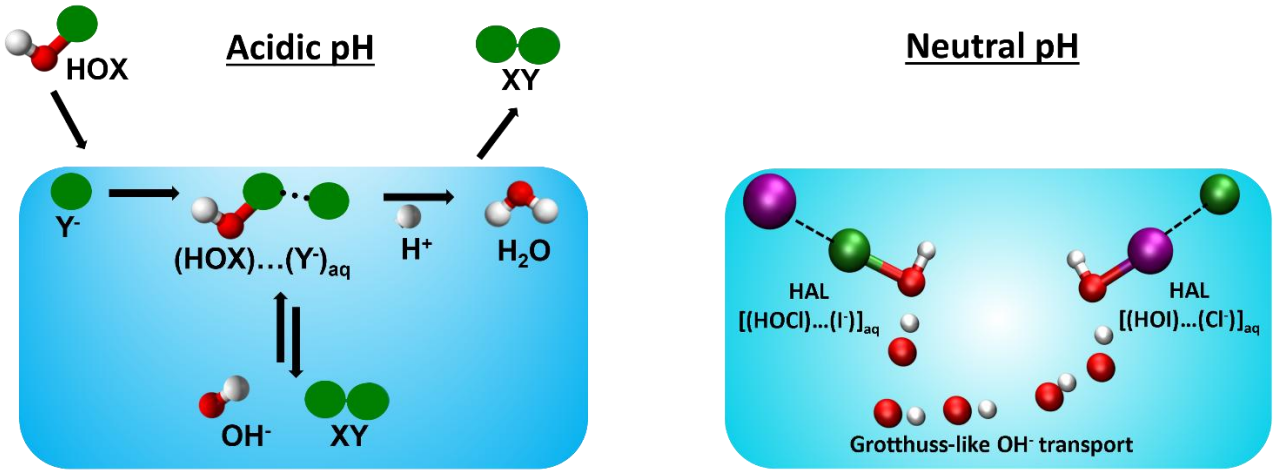


Figure 1 Dihalogen formation and halogen exchange mechanism at seawater

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Transient Occupancy and Pore Dynamics: IP6 behavior in HIV-1 T=4 Capsids

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HIV-1's genome is enclosed in a conical capsid made of capsid proteins (CA), which protects it and regulates key replication events.[1] The HIV-1 CA must maintain a balance between stability and flexibility in order to support key stages of the viral life cycle. Inositol hexakisphosphate (IP6), a negatively charged cellular metabolite, contributes to this balance by interacting with the electropositive pores of CA oligomers, particularly through coordination with residue Arg18.[2] HIV-1 capsid is not restricted to a single strict morphology. Factors like chemical cross-linking, salt concentration, or mutations can shift capsid morphology.[3,4] R18A and R18L mutations without IP6 mainly produce spherical particles, similar to T=4 icosahedrons, in high-salt conditions, showing a direct connection between R18 and capsid shape.[5,6] We performed extensive all-atom molecular dynamics simulations on T=4 icosahedral capsids in the presence and absence of IP6, as well as the R18L mutation, to gain insights into how local molecular interactions shape global capsid behavior. We find that IP6 binding to pentameric pores is energetically favorable, but the β-hairpin and R18 ring create kinetic barriers that restrict spontaneous IP6 movement, in contrast to the more accessible hexameric pores. Importantly, the local binding events, including the R18L mutation, cause minimal alterations to global capsid dynamics and ion transport. These results suggest that overall capsid geometry plays a dominant role in determining large-scale mechanical behavior, and that IP6 functions as a dynamic stabilizer rather than a strict architectural requirement.

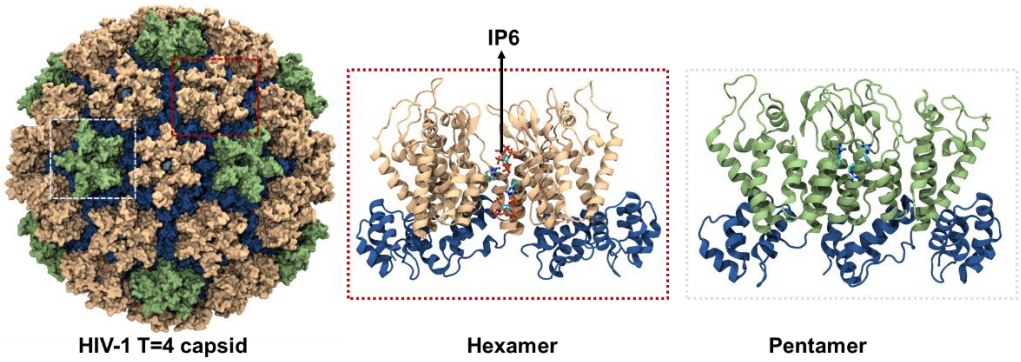


Figure 1 HIV-1 T=4 model and the representative hexamer and pentamer structures.

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Interfacial stability of Electrolytes at pure and oxidized Mg surfaces- Insights from Ab Initio Molecular Dynamics

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ABSTRACT

The development of high-performance magnesium batteries critically depends on salts that enable reversible Mg deposition. Among the leading candidates, $Mg(CB_{11}H_{12})_2$ offers excellent cycling efficiency but suffers from a high synthesis cost and impurity sensitivity. On the other hand, $Mg(TFSI)_2$, the only commercially available ether-soluble salt, undergoes electrode passivation and decomposition at Mg surfaces. Conflicting experimental and computational reports further obscure the role of surface heterogeneity on the stability of the salts. To resolve these discrepancies, we employ first-principles molecular dynamics to investigate the interfacial decomposition of $Mg(TFSI)_2$, $Mg(PF_6)_2$, and $Mg(CB_{11}H_{12})_2$ on three representative Mg anode models: pristine metallic Mg (m-Mg), stoichiometric MgO (s-MgO), and non-stoichiometric MgO (ns-MgO). We show that salt stability is strongly governed by oxide chemistry: while metallic Mg and stoichiometric MgO remain largely inert, non-stoichiometric MgO drives rapid anion decomposition and irreversible passivation. These findings establish surface heterogeneity as a key determinant of electrolyte performance and underscore the need for realistic surface models in guiding the design of next-generation Mg electrolytes.

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Fundamental Underpinnings of Ion-π Interactions: Essence and Nature

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Ion-π interactions, the noncovalent interactions between aromatic π-systems and charged species, have emerged as key contributors to a wide range of chemical and biological phenomena.[1,2] Both cation-π and anion-π interactions play critical roles in molecular recognition, catalysis, and structural stabilization.[1,2] Although these interactions are frequently rationalized in terms of the polarizability and quadrupole moment of the π-system, the (in)adequacy of such descriptors remains under active discussion.[3,4] The present study systematically examines the interactions of alkali metal cations (Li^+, Na^+, K^+) and halide anions (F^-, Cl^-, Br^-) with π-systems spanning both electron-rich (C_2H_4, C_4H_4, C_6H_6) and electron-deficient (C_2F_4, C_4F_4, C_6F_6) characters. High-level coupled-cluster calculations were employed to obtain accurate interaction energy profiles, which were subsequently decomposed into physically meaningful components, namely electrostatics, induction, and dispersion using symmetry-adapted perturbation theory.[5] We also evaluated the validity of widely used heuristic models, specifically the charge-quadrupole model for electrostatics, the charge-induced dipole model for induction, and the London equation for dispersion. The results indicate that, although the heuristic models remain valid in the long-range interaction regime, their validity diminishes as the ions approach equilibrium region or local minima. The study also reveals that, relying on the heuristic models to assess the energetics of ion-π interactions can lead to erroneous conclusions, as evidenced by the ability of some seemingly unfavourable interactions to produce metastable states and even bound states.[6,7] Overall, our study highlights the complexity of ion-π interactions and includes ongoing efforts to better understand these interactions at the fundamental level.

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Machine Learning Boosted Quantum-Profiling of Blood Antigens

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The molecular-level characterization of glycans, a challenging yet highly desirable goal, is crucial for the comprehensive advancement of glycosciences. Despite significant advances in analytical techniques, including NMR and mass spectrometry, structural and configurational complexity hinders the ability to identify carbohydrates, especially high-order saccharides with regioisomeric glycosidic linkages. Herein, we present a computational methodology that utilizes a quantum tunneling method coupled with machine learning (ML) to recognize a wide range of blood antigens simultaneously. Random forest classifier with SHapley Additive exPlanations (SHAP) interpretability performs rapid quantum profiling of all considered molecules with good precision and sensitivity. Our proposed ML-enhanced quantum methodology offers a powerful alternative to conventional techniques, facilitating accurate and high-throughput characterization of carbohydrates by performing 'sugar calling' from their transmission signatures.

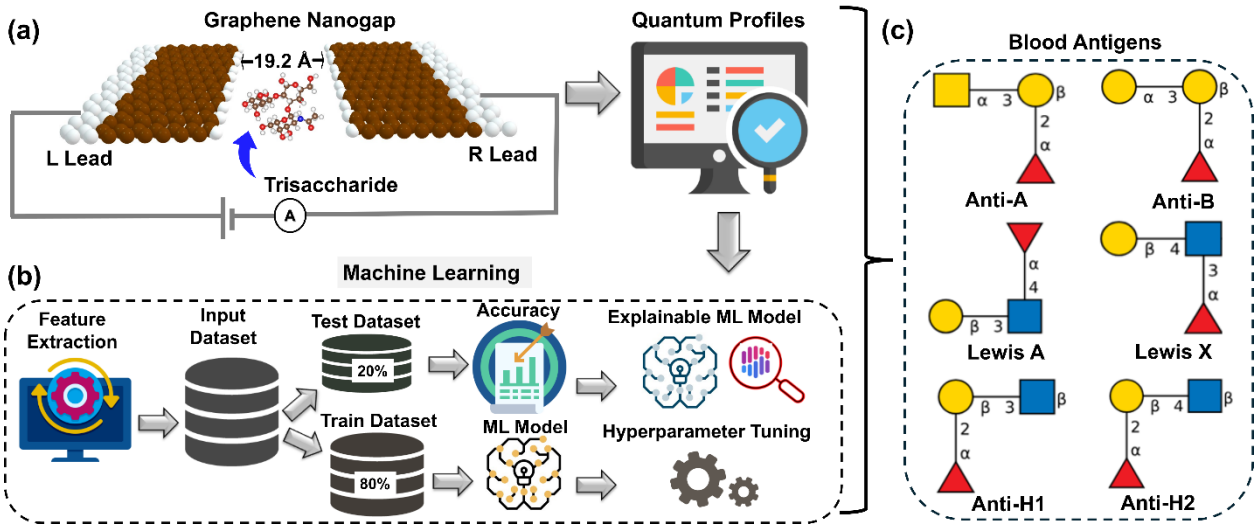


Figure 1 Schematic illustration of quantum profiling of blood antigens coupled with a machine learning (ML) workflow. (a) schematic of graphene nanogap junction in which blood antigens can be trapped in all possible orientations, (b) ML workflow for trisaccharide classification, and (c) symbol nomenclature of targeted blood antigens: Anti-A, Anti-B, Lewis A, Lewis X, Anti-H1, and Anti-H2. As per the symbol nomenclature of glycans, the yellow square represents N-Acetyl-D-Galactosamine (GalNAc), the yellow circle represents Galactose (Gal), the red triangle represents Fucose (Fuc), and the blue square represents N-Acetylglucosamine (GlcNAc).

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Unveiling the Mechanisms of Excited-State Formation in Radical-Based Organic Light-Emitting Diodes

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The emission in radical-based organic light-emitting diodes (OLEDs) originates from a spin doublet state rather than singlet or triplet excitons. In these OLEDs, the emission process is spin-allowed, circumventing the limitations imposed by triplet excitons.[1] However, some radicals typically exhibit low optical absorption and photoluminescence yields while others very emissive through the lowest first excited doublet state (D_1), making it crucial to understand the underlying mechanisms of how D_1 state is reached from the doublet ground-state (D_0) and establish design principles to enhance the absorption and luminescence yields of radical emitters.[2] Although previous studies have investigated certain processes contributing to D_1 formation[3], to the best of our knowledge, no simulations of the complete pathway from D_0 to D_1 have been conducted yet. In this study, we investigate three commonly used radical emitter molecules: TTM-1Cz, TTM-3NCz, and TTM-3PCz. These molecules share a common core structure of tris(2,4,6-trichlorophenyl) methyl (TTM) and contain varying carbazole (Cz) moieties. Using Marcus theory at the density functional level of theory (DFT), we compute the energy landscapes and barriers for multiple competitive pathways leading to D_1 formation. We also examine the validity of Marcus theory for such complex systems, particularly in regimes where quantum effects such as tunneling may become significant, especially in the inverted Marcus regime. The pathways analyzed include: i) D_1 formation via radical-anion intermediate, ii) D_1 formation via radical-cation intermediate, iii) D_1 formation via charge-charge annihilation, and iv) D_1 formation via higher-lying doublet or quartet states.[4] This in-depth DFT-based analysis of competitive pathways provides critical insights for designing next-generation radical emitters with improved efficiency and performance.

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Theoretical Chemistry Symposium
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A Computational Study on cis–trans Photo and Thermal isomerizations of Azobis(benzo-15-crown-5) and its Metal Ion Complexes

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Computational studies on the thermal and photo-induced cis-trans isomerizations of photoresponsive azobis(benzo-15-crown-5) have been carried out (Figure 1). For the trans isomer, the photoexcited ππ* (S_2) state relaxes via a planar minimum and a planar S_2/S_1 conical intersection along the N=N stretching coordinate, while the nπ* (S_1) state features both planar and rotational minima, where the latter leads to a torsional S_0/S_1 conical intersection with a CNNC dihedral angle value close to 90°. The rotational pathway exhibits an energy barrier which is lowered through a coupled N–N out-of-plane motion, facilitating the trans→cis isomerization. In contrast, the cis isomer undergoes barrierless photoisomerization along the S_1 surface via a torsional S_0/S_1 conical intersection, where as the S_2/S_1 CI lies too high in energy to be accessed upon ππ* excitation. Thermal cis → trans thermal isomerization proceeds through an inversion pathway forming a less stable trans form. The rotational counter part of this pathway requires more barrier, however, along this route a non-adiabatic singlet-triplet (S_0/T_1) crossing has been noticed which opens a comparatively easier cis→trans conversion pathway. In recent times, we have performed alkali metal-initiated isomerization processes of this crown ether which is related to the ion transport phenomenon. Presence of counter anion is found to influence these isomerizations as it eases the opening of the cis form which subsequently undergoes a conical intersection (S_0/S_1) to form the trans isomer.

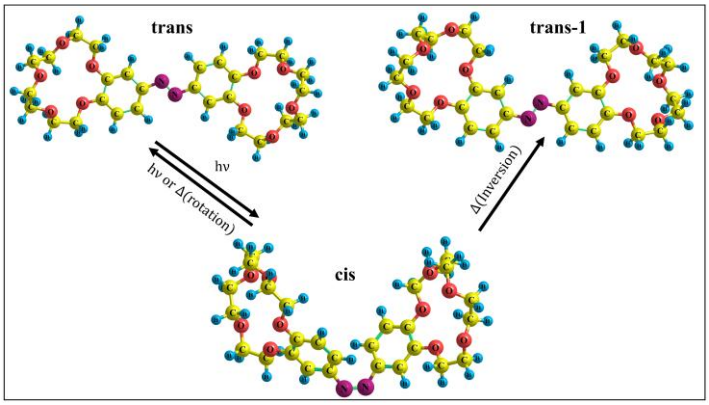


Figure 1. Thermal and photo-induced isomerizations of photoresponsive azobis(benzo-15-crown-5)

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Second-Order Saddle Points and Concerted Reaction Mechanism: Insights from Entangled Trajectory Molecular Dynamics

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Reactions involving complex networks of transition states—such as those featuring bifurcations or higher-order saddles—require a molecular dynamics framework for accurate mechanistic insight. Quantum effects are crucial in certain regimes, but accounting for them remains challenging, especially for high-dimensional complex systems. A promising method in this context is the entangled trajectory molecular dynamics (ETMD) technique by Martens and coworkers[1], which employs quantum trajectories in phase space using Wigner distribution.

In this work, we apply ETMD to a two-degree-of-freedom Hamiltonian model[2] of double proton transfer, characterized by four minima, four rank-one saddles, and a rank-two saddle—providing a rich topological framework for mechanistic analysis. Guided by studies on higher-order saddles[3], we use Houk's delay time concept[4] to compare classical and quantum pathways and identify concerted dynamics. We observe significant fluctuations in the fraction of concerted trajectories even at energies above the second-order saddle. Notably, ETMD identifies energy regimes where classical trajectories become dynamically trapped, while quantum trajectories exhibit barrier-crossing behavior indicative of dynamical tunneling. These quantum pathways are further analyzed using Lagrangian descriptors[5] and entanglement entropy[6], offering a phase-space interpretation of quantum-enhanced concertedness.

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Theoretical Chemistry Symposium
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Different Water Architecture Diversifies the Catalytic Activity in Two Deceptively Similar Cytochrome P450 Isozymes

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Abstract

Cytochrome P450 (CYP450) enzymes are ubiquitous in nature, and they catalyze a plethora of biologically relevant reactions in all sorts of biological kingdoms. It uses molecular oxygen and inserts it into the incoming substrate during oxidation of the substrate [1]. Among several members of the Cytochrome P450 enzymes, CYP1A1 and CYP1A2, are pivotal in the bioactivation of polycyclic aromatic hydrocarbons (PAHs), converting them into carcinogenic metabolites [2]. Although both enzymes exhibit structural adaptation to bind PAHs and possess very similar protein structures, they show differential reactivity with α-naphthoflavone (ANF), a known CYP1 family inhibitor. CYP1A1 demonstrates minor metabolic activity toward ANF, while CYP1A2's reaction is almost negligible [3]. To investigate the mechanistic underpinnings of this selective metabolism, we perform molecular dynamics (MD) simulations and hybrid quantum mechanics/molecular mechanics (QM/MM) calculations, examining structural dynamics and electronic factors within the active sites of CYP1A1 and CYP1A2. The MD simulation of both enzymes in the presence of the ANF shows different water organization in the two enzymes. The CYP1A1, which shows metabolic activity, forms an organized water channel stretching from the ANF to the heme iron-oxo, enabling substrate oxidation via the Grotthus mechanism. While such organization was missing in CYP1A1 which is the root cause of the loss of the activity. The study provides a mechanistic insight that could help to design selective CYP1 inhibitors, contributing to strategies for mitigating PAH-related carcinogenicity by fine-tuning enzyme specificity.

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Unlocking Inverted Singlet–Triplet Gap in Alternant Hydrocarbons with Heteroatoms

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With the growing interest in diverse material systems for organic light emitting diodes (OLEDs), multiresonant thermally activated delayed fluorescence (MR-TADF) compounds have attracted considerable attention due to their unique photophysical properties and efficient triplet harvesting. Building on these developments, we explore boron–nitrogen-substituted polycyclic aromatic hydrocarbons (BNPAHs) as promising candidates for fifth-generation OLEDs[1]. These next-generation materials rely on delayed fluorescence from inverted singlet and triplet states (DFIST), where the first excited singlet lies below the triplet, enabling exothermic reverse intersystem crossing. Previous DFIST studies have focused on triangular anti-aromatic cores, which often suffer from structural instability[2]. In our earlier work, we also showed that such Hund's rule-violating systems are absent in the small-molecule chemical space[3]. A recent study extended this search to heteroatom-doped PAHs and found small singlet–triplet gaps[4], though none with true inversion. In this work, we go further to systematically investigate a large aromatic space of 30,797 BNPAHs derived from 77 scaffolds. Using a multi-step workflow combining stability checks and accurate excited-state calculations, we identify 46 robust candidates with negative singlet–triplet gaps. Notably, some exhibit inversion via through-space charge transfer and feature non-planar helicenes, expanding the design space for efficient, stable, metal-free OLEDs.

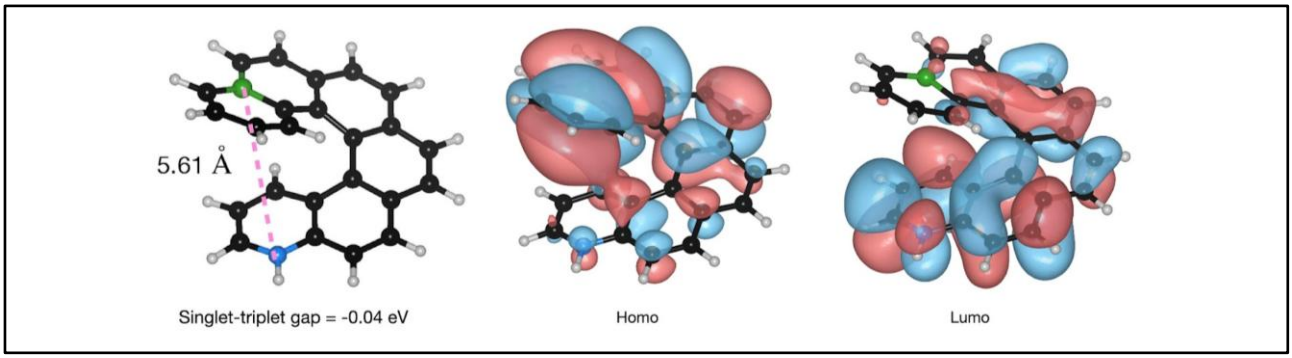


Figure 1: B,N-hexahelicene with a negative singlet-triplet gap[1]

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Cellular uptake of microgels by membrane wrapping

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The interaction of nano- and microparticles with lipid-bilayer membranes plays a key role in the process of cellular engulfment.[1] The physico-chemical parameters that control engulfment are size, shape, elasticity of the particle, and bending rigidity, tension of the membrane, and particle-membrane adhesion strength.[2] Stimuli-responsive polymeric microgels are particularly versatile because their elasticity can be tuned in a wide range by changing the density of crosslinkers. Using continuum models of spring networks for the microgels, and triangulated surfaces with Helfrich's curvature elasticity for the membrane, we study microgels wrapping at lipid-bilayers,[3] where microgels are attached to the membranes via ligand-receptor bonds. Hertz theory is employed to characterize the microgel's Young's modulus and Poisson's ratio. The interplay of microgel and membrane deformations is controlled by the competition between microgel elasticity and membrane bending rigidity. Our numerical simulations predict an increased stability of partial-wrapped states for microgels at lower Young's moduli. There is a discontinuous transition from oblate to nearly spherical microgels with increasing wrapping fractions, irrespective of membrane tension. Volume and surface area of partial-wrapped microgels are significantly reduced compared with those of free microgels.[3] Understanding microgel wrapping will facilitate the design of tunable and responsive polymeric gels for biomedical applications, e.g., targetged drug delivery vectors.

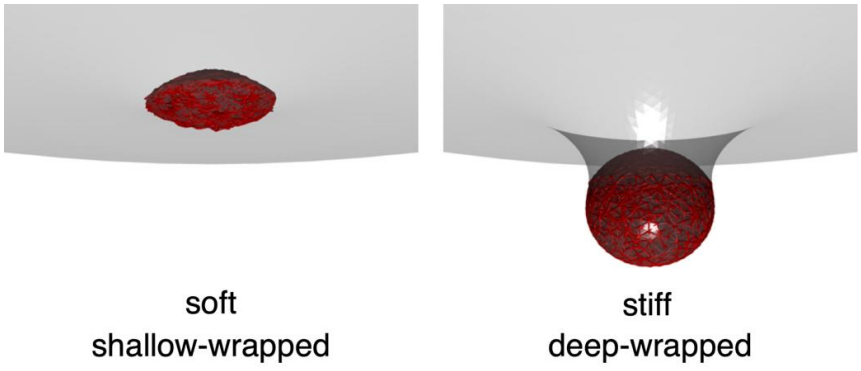


Figure 1 Stable wrapping states for soft and stiff microgels with same adhesion fraction

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Learning Condensed Graph via Differentiable Atom Mapping for Reaction Yield Prediction

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Predicting the yield of a chemical reaction is a fundamental challenge in chemistry. A key determinant of yield is the transition state, a transient high-energy structure. Existing deep learning models often overlook this critical aspect as real-world datasets typically lack any transition state(TS) information. To address this, we introduce YieldNet, a neural network that first approximates atom mapping using a differentiable node alignment module[2], allowing it to estimate a continuous condensed graph(CGR)[1] of the reaction as a surrogate transition state. This surrogate graph is then processed by input-differentiable graph neural networks and a transformer-based reaction path encoder to predict yields across multi-step reactions. Crucially, the model is trained solely under the distant supervision of reaction yield values, without requiring ground-truth atom mappings or transition states. This enables end-to-end learning of chemically meaningful inductive bias from data alone. This work bridges a key gap between physical chemistry and machine learning, offering a practical tool for chemists to screen and optimize reactions more effectively. YieldNet could accelerate discovery in fields ranging from pharmaceuticals to materials science by reducing the need for costly lab experimentation.

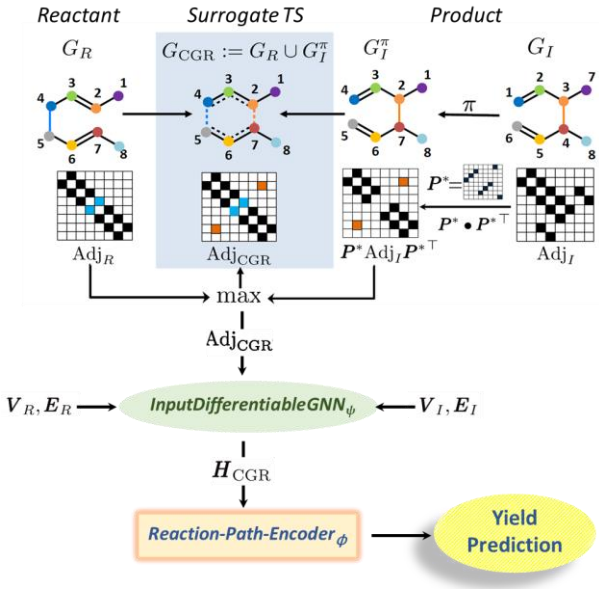


Figure 1 Illustration of YIELDNET. For each reaction step, we feed the node embeddings and edge embeddings into a fully differentiable node alignment network to obtain an alignment matrix P which gives a continuous approximation of the adjacency matrix of CGR, $\mathrm{Adj}_{\mathrm{CGR}}$ and feed this approximate $\mathrm{Adj}_{\mathrm{CGR}}$ with the node and features into a new GNN to obtain H_{CGR}, the node embedddings of CGR. Finally, a reaction path encoder use $\{H_{\mathrm{CGR}}\}$ to predict the yield.

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Exploring How Metal–Oxo Identity (Fe, Co, Mn) Governs C–H Activation in Ethylene-Forming Enzymes

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Abstract: The selective activation of aliphatic C–H bonds remains a central challenge in catalysis due to their inertness and high bond dissociation energies.[1-3] Among biological systems, nonheme Fe(IV)=O species have emerged as key oxidants capable of promoting such transformations, notably in ethylene-forming enzymes (EFEs), where they facilitate L-arginine oxidation via efficient C–H activation.[3] In this study, we investigated the effect of metal substitution in EFEs by replacing iron with cobalt and manganese to understand how metal identity influences catalytic reactivity. Through extensive molecular dynamics (MD) simulations, we probed the structural flexibility and stability of the Fe, Co, and Mn variants. Local Electric field (LEF) analyses were conducted to quantify protein-generated local electrostatic effects during the trajectory and in key intermediates. Hybrid QM/MM calculations were employed to map out the energy landscapes and spin-state preferences across metal-substituted systems. Furthermore, multireference CASSCF calculations revealed significant differences in spin-state mixing and wavefunction character, providing insights into the electronic factors that govern C–H bond activation efficiency. Our findings establish a strong correlation between electric field directionality, spin-state energetics, and reactivity, offering a comprehensive understanding of how metal substitution modulates catalytic behavior in EFE-like systems.

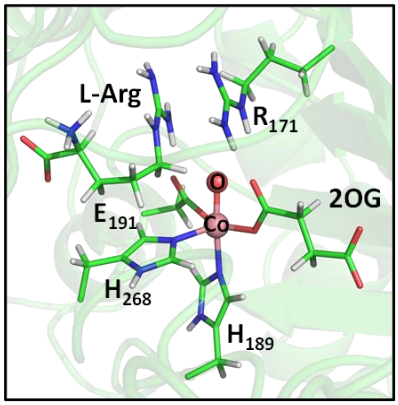


Figure 1: Representative MD-derived structure of the Co^{IV}=O species in EFE, highlighting Glu_{191}, His_{268}, His_{189}, 2-α-ketoglutarate, L-arginine (substrate), and Arg_{171}, with Arg_{171} forming a hydrogen bond to the oxo group of Co^{IV}=O.

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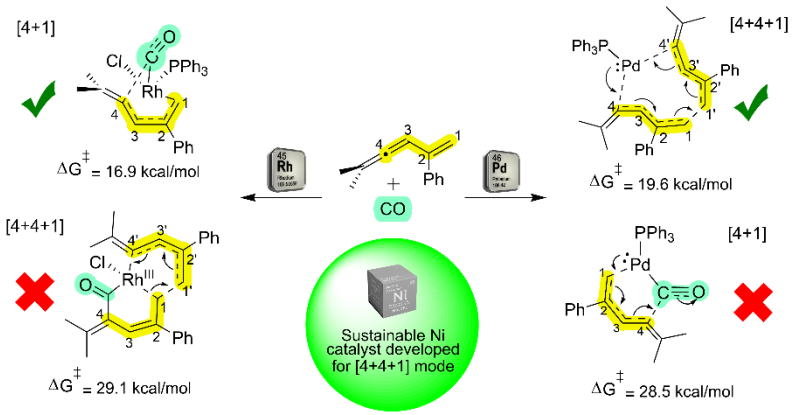
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Why Does Rh Prefer [4 + 1] while Pd Prefer [4 + 4 + 1] Mode in Carbocyclization of Vinylallene with CO? Unveiling Nickel's Potential for Expanding the Scope Beyond Pd

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Rhodium(I) promotes a [4 + 1] assembly mode with a vinylallene substrate and CO, leading to the formation of a five-membered ring structure. In striking contrast, palladium(0) catalyzes a more complex [4 + 4 + 1] mode leading to a nine-membered cyclic ketone. The underlying mechanisms that govern this contrast in assembly modes remain unclear, even in today's date, presenting a major challenge to the further development of efficient reactions. Our computational study[1] reveals that Rh adopts a square pyramidal geometry with CO. This is in contrast to Pd, which prefers a trigonal planar geometry. A stronger metal–CO interaction is detected in Rh than in a Pd intermediate, making the [4 + 1] mode more preferable in Rh than in Pd. The transition state for C–C coupling between two vinylallene has a significantly distorted tetrahedral core in the case of Rh, while Pd retains a stable trigonal planar structure, making the [4 + 4 + 1] reaction less favorable in Rh than in Pd. By conceptualizing and transferring the critical features of Pd to Ni systems, we have rationally designed a Ni-catalyzed [4 + 4 + 1] version that combines the desirable reactivity of Pd with the cost-effectiveness and abundance of Ni, aligning with the growing demand for more sustainable and atom-efficient strategies in synthetic organic chemistry.



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EFFECT OF GLYCOSYLATION ON THE CONFORMATIONAL DYNAMICS OF THE CATALYTIC DOMAIN OF HUMAN CARBONIC ANHYDRASE IX

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The enzyme human carbonic anhydrase IX (HCA IX) is a multi-domain, dimeric protein. Glycosylation of its catalytic domain has been linked to its unique role in promoting the survival of malignant cells of solid tumors under low pH conditions. In the present work, we probe the role of glycosylation in terms of possible coupling of conformational fluctuations of the glycan chain to functionally important dynamics of the enzyme.[1] In the glycosylated monomeric and dimeric forms of the catalytic domain of HCA IX (HCA IX-c), the glycan chain is predominantly found in an extended conformation oriented towards the bulk solvent. In some rare conformations, the glycan chain back-folds towards the protein surface and transiently forms hydrogen bonds to surface-exposed polar amino acid residues of the protein. Few such back-folded structures connect to the reactive proton transfer pathway via Glu-106, as shown in Figure 1.[2] In dimeric HCA-IX-c, the two glycan chains simultaneously form the rare backfolded and half-backfolded conformations. The observed correlation between glycan chain fluctuations and the reorganization dynamics at the active site is further investigated to reveal allosteric cross-talks[3] between the glycan chain and His-64, critical for catalysis. From free energy disconnectivity graphs (FEDs), we identify distinct conformational basins corresponding to active and allosteric states and analyze the correlated accessibility of distant substates indicating an allosteric coupling.

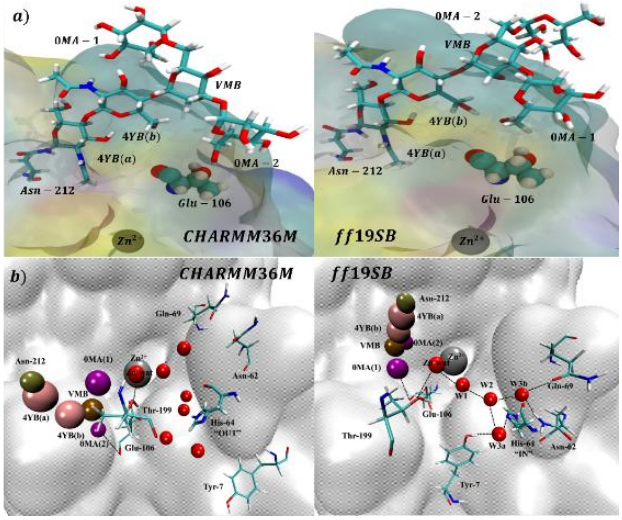


Figure 1: (a) Back-folded glycan chain conformations. (b) Transient proton transfer network when the glycan chain is in two different back-folded conformations.

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B−B Sites in Molten Boron Oxide are Superior to Cyclic B−O−B Sites for Methane Oxidation to Formaldehyde and Carbon Monoxide

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Boron oxide (B_2O_3) is a promising metal-free catalyst for the oxidative dehydrogenation (ODH) of methane, yielding high selectivity for formaldehyde (HCHO) and carbon monoxide (CO) at 823 K. Since the reaction occurs above the melting point of B_2O_3 (~725 K), it likely proceeds in the molten state. Building on our earlier work on methane ODH over crystalline boron oxide[1,2] and hexagonal boron-nitride[3]. Here, we present a detailed DFT-based mechanistic study of methane oxidation over these structural motifs with $^1O_2$ and $^3O_2$.[4] The results identify the B−B site as the most catalytically active motif for HCHO formation, requiring a low activation barrier of 36.6 kcal mol^{-1}. In contrast, cyclic B−O−B motifs exhibit substantially higher barriers (~50–78 kcal mol^{-1}). Orbital analyses highlight distinct electron transfer pathways: oxygen lone-pairs in B−O−B rings, versus σ(B−B) bond donation at B−B sites. Additionally, CO formation is predicted to be thermodynamically more favorable than CO_2, consistent with existing experimental trends.

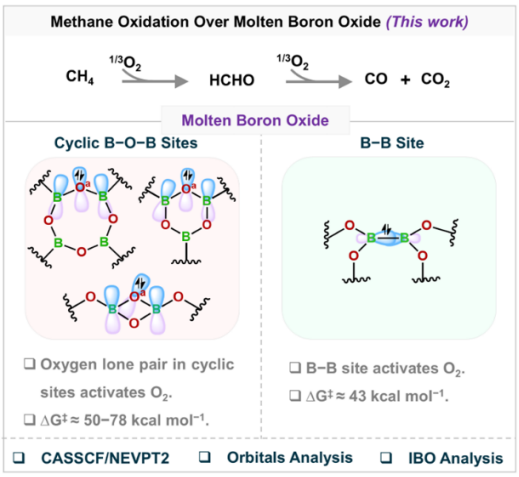


Figure 1 Oxidative Dehydrogenation of Methane over Molten Boron Oxide

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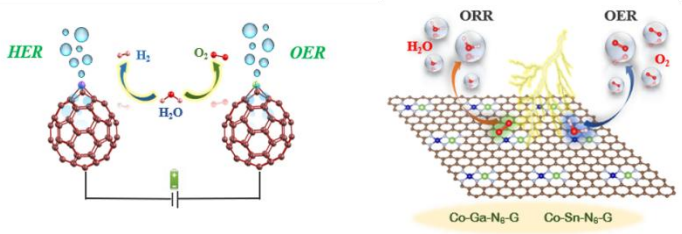
Computational Modelling of metal doped carbon nanostructures for electrochemical water splitting and metal air battery applications

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The growing demand for sustainable energy has intensified the search for efficient and cost-effective electrocatalysts for water splitting and metal-air batteries, particularly due to the adverse impacts of fossil fuels. Single- and bi-atom catalysts have emerged as highly promising candidates for key electrochemical reactions such as the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR).

In this poster, we present the catalytic applications of transition metal (TM)-doped carbon-based nanostructures, specifically graphene and fullerene for renewable energy applications. Using density functional theory (DFT), we investigate TM doped (Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt) fullerene as electrocatalyst for water splitting.[1] The results indicate that sixth-row TMs, particularly Ir and Pt, exhibit outstanding HER activity, while fifth-row metals such as Ru and Pd show superior performance in OER. In a separate study, the bifunctional electrocatalytic performance for metal air battery is examined for TM (Fe, Co, Ni) co-doped nitrogen-doped graphene systems (TM-N_6-G) by introducing p-block metals (PM = Al, Ga, In, Sn, Bi) into an N_4 cavity, resulting in TM-PM-N_6-G structures.[2] Systematic DFT calculations reveal that Co-Ga-N_6-G and Co-Sn-N_6-G configurations exhibit remarkable bifunctional catalytic performance for OER and ORR, with several others unifuncional catalysts. The Co centers act as the active sites for OER/ORR, while the PM atoms play a crucial role in enhancing the catalytic activity of the transition-metal centers.

The enhanced catalytic activity is attributed to optimal interactions with reaction intermediates, as supported by scaling relations and volcano plots. The influence of the electronic structure is elucidated through band-center and COHP analyses, charge distribution on the metal centers, and contour maps. Furthermore, correlation functions are analyzed to propose a new descriptor for designing efficient bifunctional catalysts. Thermal stability of the most promising catalysts is assessed using AIMD simulations.



(a) (b)

Figure 1: (a) Transition-metal-doped fullerene exhibits efficient electrocatalytic water splitting activity. (b) p-block and transition metal-doped N-graphene demonstrate bifunctional electrocatalytic activity for OER and ORR.

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Beyond Red: Uncovering New NIR-TADF Emitters One Bit at a Time

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Near-infrared (NIR) thermally activated delayed fluorescence (TADF) materials are emerging as critical components in technologies ranging from organic light-emitting diodes to bioimaging and photodynamic therapy. Despite their promise, the rational design of efficient NIR-TADF emitters remains hindered due to limited diversity in known acceptor motifs and the inherent energy-gap law, favoring non-radiative pathways at lower energies. In this work, we introduce a machine learning (ML)-guided strategy to accelerate the discovery of novel NIR-TADF candidates by leveraging the rich structural diversity of non-fullerene acceptors (NFAs). Through interpretable fingerprint-based modeling, we identify substructures responsible for red-shifted absorption and strategically recombine them with TADF donor motifs to generate a diverse molecular library. Our method integrates quantum-chemical methods with data-driven feature analysis to pinpoint fragment-level design rules that promote long-wavelength emission. This framework not only offers a sustainable and cost-effective path for navigating unexplored regions of chemical space, but also paves the way for data-efficient inverse design of next generation NIR-TADF emitters.

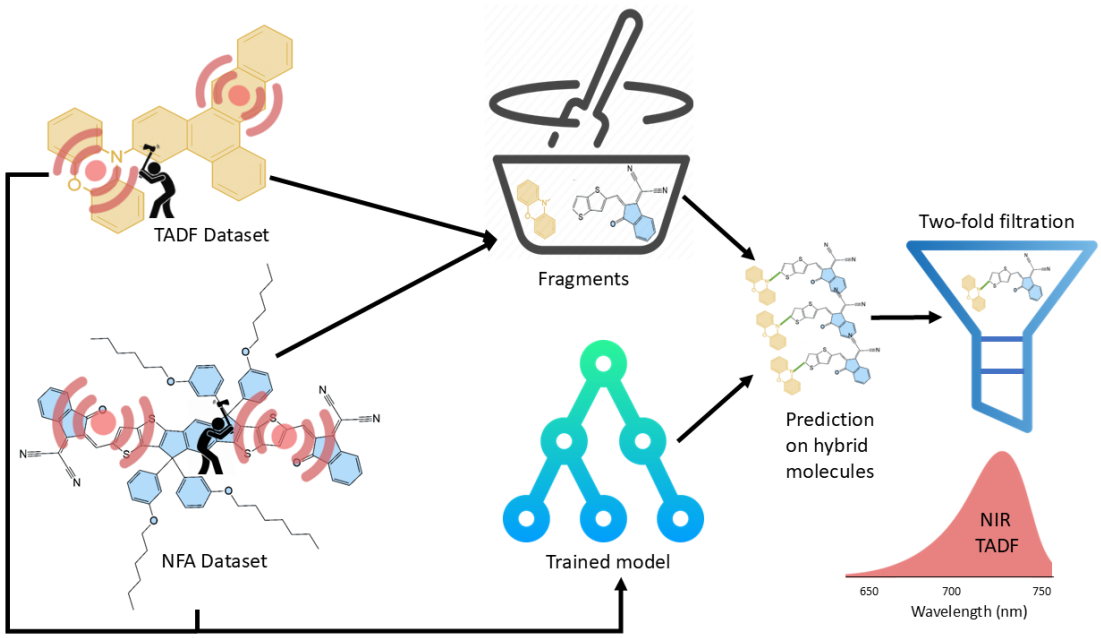


Figure 1 A schematic representation of the workflow implemented in this study.

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Machine Learning of Thermodynamic Ergotropy in Cavity-Mediated Quantum Batteries

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Abstract

Optimizing quantum-battery performance that leverages through quantum coherences and depend upon parameter optimisation and thermodynamic quantities like ergotropy (ε), proves challenging in open systems where populations and coherences are intrinsically coupled. Here, we study a four-level cavity-mediated quantum battery using quantum master equations combined with hybrid machine learning to identify optimal operating regimes. Feature importance analysis followed by testing revealed a minimal four-parameter subset-kurtosis $C^{(4)}$, cold bath coherence strength (p_c), temperature of the hot reservoir (T_h), and heat input (Q_h) that attains an accuracy of 0.90. Expanding to eight parameters by adding heat output (Q_c), leak reservoir temperature (T_l), first excited state energy (ε_b), and second excited state energy (ε_a) yielded an accuracy of 0.98. The four-parameter option offers practical advantages, since collecting four measurements is significantly easier than obtaining eight distinct parameters in experimental or computational quantum battery systems. These results indicate that path-induced coherences can enhance work extraction beyond classical limits and offer flexibility between minimal and comprehensive protocols for quantum energy storage optimization.

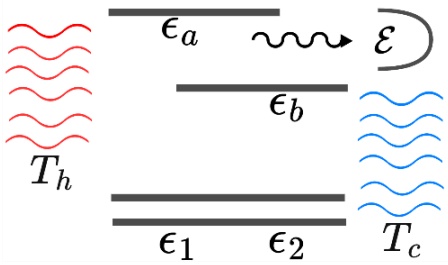


Figure 1. Schematic representations of the quantum-battery model showing coupling to hot and cold reservoirs.

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Theoretical Chemistry Symposium
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Polynomial Scaling Localized Active Space Unitary Selective Coupled Cluster Singles and Doubles

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We present a polynomial-scaling algorithm for the localized active space unitary selective coupled cluster singles and doubles (LAS-USCCSD) method. In this approach, cluster excitations are selected based on a threshold ϵ determined by the absolute gradients of the LAS-UCCSD energy with respect to cluster amplitudes[1,2]. Using the generalized Wick's theorem for multireference wave functions, we derive the gradient expression as a polynomial function of one-, two-, and three-body reduced density matrices and 1- and 2-electron integrals, valid for any multireference wave function[2]. The resulting gradient implementation exhibits a memory scaling of $\mathcal{O}(N6)$, with N_{spin} orbitals in the combined active space of all fragments. The variational quantum eigensolver is used to optimize the selected cluster excitations on a quantum simulator. By plotting the energy error, defined as the difference between the LAS-USCCSD and corresponding CASCI energies, against the inverse cluster amplitude selection threshold (ϵ^{-1}) for polyene chains containing 2 to 5 π-bond units, we establish a relationship between the energy error and the threshold. To further validate the accuracy of LAS-USCCSD, we computed the cis–trans isomerization energy of stilbene (a 20-qubit system) and the magnetic coupling constant of the tris-hydroxo-bridged chromium dimer $[Cr_2(OH)_3(NH_3)_6]^{3+}$ (evaluated as both 12- and 20-qubit systems) using the Qiskit-Qulacs simulator. Assessing such examples is important to determine the practical feasibility of quantum simulations for chemically realistic systems. Toward this goal, with the LAS-USCCSD algorithm we estimated the quantum resources required for simulating an active space of (30e,22o) in $[Cr_2(OH)_3(NH_3)_6]^{3+}$, a size that remains beyond the reach of current quantum simulators for accurate treatment.

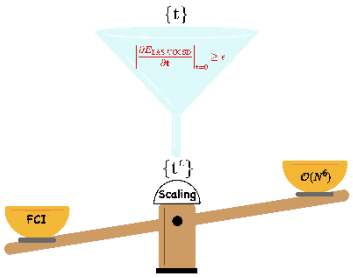


Figure 1: The polynomial scaling LAS-USCCSD algorithm is computationally more efficient than an FCI-based exponential scaling algorithm.

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Ab Initio Modelling of Spin Relaxation in Metal-Organic Framework-based Qubits

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Molecular qubits based on extended coordination frameworks represent one of the latest frontiers of spin-based quantum sensors or qubits, where long spin coherence times are combined with chemical versatility. The electronic states and vibrational modes of these frameworks carry sufficient information, which eventually exhibit long coherence time to behave as qubits. Here we employed ab initio spin relaxation theory to fully investigate the role of one- and two-phonon processes to understand the spin-phonon relaxation of vanadyl tetraphenylporphyrinate MOF, namely in [VO(TCPP-Zn_2-bpy)].[1] Here, we used the ab initio spin relaxation theory[2] to simulate the spin-lattice relaxation time (T_1) using NEVPT2(1,5) and NEVPT2(9,9) methods. Expanding the active space from d-d excitations to metal-ligand bonding orbitals[3] clearly shows an improvement in the spin-dynamics, emphasizing the use of the full electronic Hamiltonian instead of the effective Hamiltonian formalism, where the latter is often used as a standard method in lanthanide complexes.

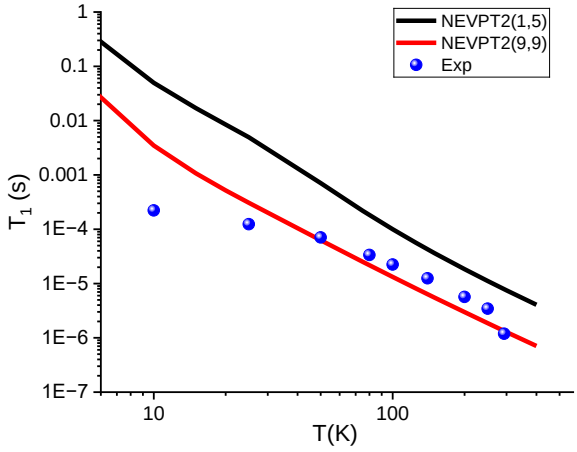


Figure 1 Comparison of the experimental and ab initio spin-lattice relaxation time (T_1) for the VOTCPP MOF using different active spaces.

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Evaluating the preferential adsorption of N_2 from a binary mixture of N_2/O_2 on extra-framework cations of zeolites: a computational and experimental study

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Separation of N_2 from a N_2/O_2 gas mixture is critical for various industrial/medical applications. Temperature/pressure swing adsorption is the top-notch industrial technology used for this separation, where zeolites are the materials used for adsorption. Zeolite X/Y with Li^+ as an extra-framework cation is the best-known sorbent for N_2 gas molecules. However, the present net-zero emission scenario has made lithium a critical element, making it imperative to implement its alternative in various other technologies. In this context, the present work is a computational evaluation to identify a cation that can replace Li^+ for preferential adsorption of N_2 over O_2. The DFT study, based on parameters such as selective adsorption energies of N_2 over O_2 and IR stretching frequencies of the adsorbed N_2 and O_2 molecules, identifies Mg^{2+}, Ca^{2+}, Sr^{2+}, Co^{2+} and Zn^{2+} as potential cations. These cations have preferential adsorption for N_2 over O_2 by 10 kJ mol^{-1} or more. However, BOMD simulations reveal that only Mg^{2+}, Ca^{2+}, Co^{2+} and Zn^{2+} keep the N_2 molecule bound at 300 K, and the O_2 molecule gets desorbed from these frameworks. The desorption temperature of N_2 on Ca^{2+} and Zn^{2+} is 350 K, and on Mg^{2+} is 400 K. These observations are corroborated by electronic charges on cations and molecular orbitals. Significantly, Ca^{2+} is identified to adsorb up to 2 N_2 molecules, making it an ideal candidate for N_2/O_2 separation in place of Li^+. To validate this, we have carried out an experimental study that showed a good N_2 adsorption capacity of 2.1 mmol g^{-1} for Ca^{2+}.

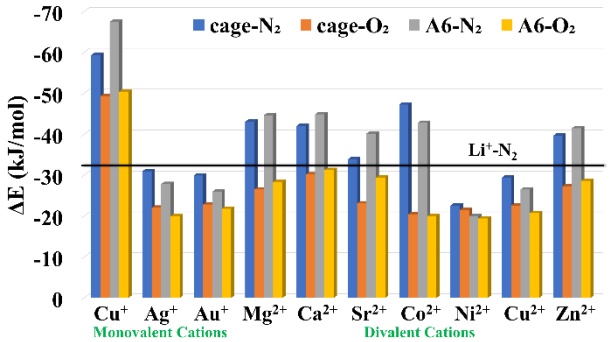


Figure 1 Adsorption energy (in kJ/mol) of the N_2 and O_2 molecules on various cation exchanged sodalite cage and A6 cluster models. The black line passing through the graph is the adsorption energy value of the N2 molecule adsorbed on the Li^+ ion.

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Theoretical Chemistry Symposium
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Hydrophobic Collapse and Mechanical Forces in β-Hairpin Folding-Unfolding

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Proteins must fold into precise three-dimensional structures to function effectively. While much is known about the role of internal interactions during folding like hydrophobic collapse, the influence of very subtle forces[1] of the order of pico-newtons remains unexplored.In this work, we employed molecular dynamics coupled with enhanced sampling to study the folding-unfolding of the TrpZip2 β-hairpin and the Small Protein under varying force conditions. Further we examined the effects of hydrophobic interactions, and external perturbations on the folding-unfolding pathway. We converge to the conclusion that a force of ~5 pN along the backbone aids in stabilizing the native state, while deviation from this value destabilize the protein. The non-uniform forces from hydrophobic collapse, particularly of tryptophan residues, act as a natural directional pull guiding the backbone into its proper conformation[2]. Simulations with an external 5 pN force confirm that such a small pull is sufficient enough to bias the folding landscape toward the native state. We propose that tryptophan residues can exert an intrinsic force of this order on the peptide backbone. These insights suggest ways to design force-clamp experiments for stabilizing secondary structures.

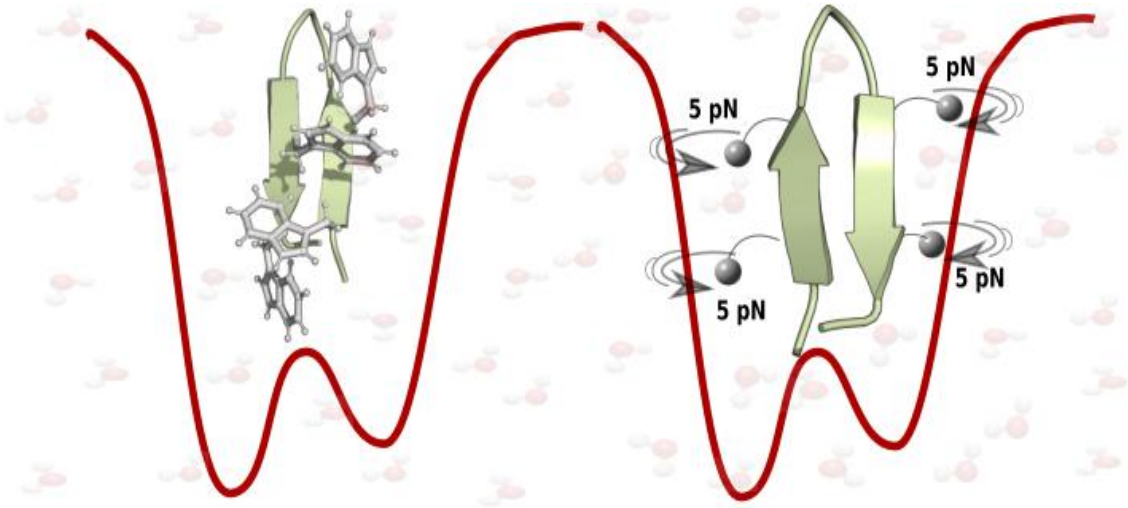


Figure 1 Free energy profile of a β-hairpin in the presence of tryptophan residues and under an applied 5 pN force.

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Valence Isomerism in Biological Iron-Sulfur Clusters

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Iron-Sulfur clusters are vital for electron transfer and catalysis of biochemical processes in all forms of life, from bacteria and plants to animals.[1] They are challenging to study due to their core's (Fe_4S_4) complex electronic structure and high density of spin states. However, both of these factors are considered key to their rich chemistry.[2] Iron–sulfur clusters in proteins often exhibit antiferromagnetic coupling, where individual iron centers couple through bridging sulfides to yield a net low-spin ground state.[3] In the widely used *pairs-of-pairs* model for Fe_4S_4 clusters, the four irons form two strongly antiferromagnetically coupled Fe–Fe pairs, allowing multiple valence isomers depending on how charges are distributed across the pairs. For instance, a mixed-valence Fe(II,III) pair of high-spin ions with spin S = 9/2 and a ferrous Fe(II,II) pair of spin S = 4 are coupled antiferromagnetically to give an overall low-spin ground state (S = 1/2), which exhibits a characteristic EPR signal.[4] In the case study of Fe_4S_4 cluster in [Fe-Fe] hydrogenase using MD simulations and QM/MM techniques we found that valence isomerism between $Fe^{2.5+}$ and Fe^{2+} pairs is strongly affected by the flexibility of second coordination sphere residues (Arg227 and Lys228) thereby influencing the cluster's electronic structure and potentially its catalytic properties.[5] These results are used to understand EPR observations on the enzyme. These findings highlight the interplay between valence localization, protein environment, and structural flexibility in biological Fe–S clusters.

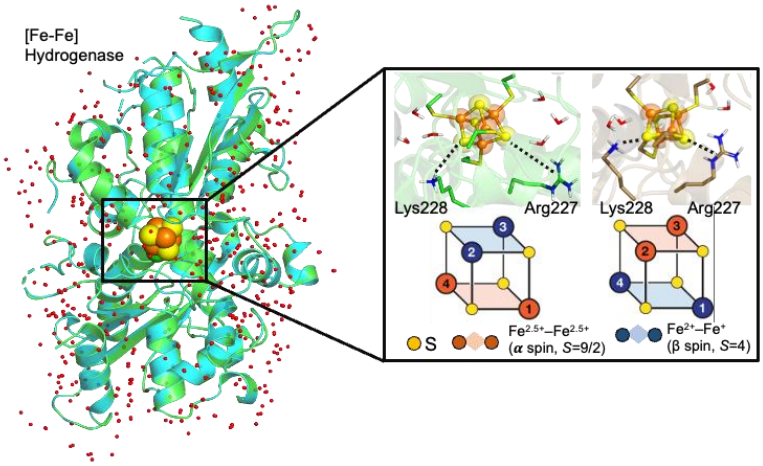


Figure 1 Schematic depiction of the valence isomers obtained by QM/MM calculations on the different configurations of Fe_4S_4 cluster.

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Molecular Insights into Solvation Structures and Ion Transport Mechanisms in Glyme-Based Electrolytes for Potassium-Ion Batteries

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The growing demand for safer and more efficient energy storage devices has led researchers to investigate alternatives to Li-ion batteries. Potassium (K) emerged as a promising candidate for next-generation energy storage devices due to its small stokes radius, high negative redox potential, and, most importantly, it does not form an alloy with aluminum.

Despite many advantages, the high reactivity of potassium shows significant challenges, including uncontrolled side reactions and unstable solid electrolyte interphase (SEI) at interfaces, resulting in low cycle life and capacity fading. To encounter these issues, researchers investigate different combinations of salts, solvents and additives in electrolytes. The solvation structure and dynamics[1-3] of the electrolyte plays a crucial role in determining the performance and smooth functioning of the battery.

We employ a combination of MD simulations and DFT to gain deeper insights into the solvation structures and electrochemical stability windows of glyme-based electrolytes. In this study, we systematically investigate the effect of glyme chain length on solvation environments and their influence on electrolyte properties. A comprehensive structural and dynamical analyses was carried out to elucidate the behavior of different electrolyte compositions. Statistical evaluation of solvation structures provided a clear understanding of the underlying ion transport mechanisms operating in these electrolytes. Furthermore, cage dynamics and potential of mean force calculations revealed the nature and strength of ion–solvent and ion–ion interactions, offering molecular-level insights into the transport and stability of glyme-based electrolytes for potassium-ion batteries. Figure 1 illustrates the chemical components used in the preparation of electrolytes.

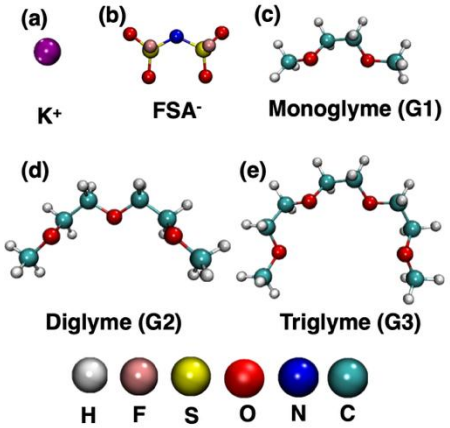


Figure 2 Chemical structure of molecules and ions used in this study.

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Unveiling the activity and selectivity of single metal atom supported on AlN monolayer for electrochemical conversion of NO to NH_3: A DFT study

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Electrochemical nitric oxide reduction reaction (NORR) is a promising alternative method to capture and utilize NO, emitted due to the massive acceleration of the nitrogen cycle resulting from various human activities[1]. In this study, the NORR catalytic performance of a series of single transition metal (M) atoms anchored on two-dimensional aluminium nitride (AlN) monolayer, *i.e.*, M@AlN (named single-atom catalyst (SAC)), is performed by using spin-polarised density functional theory (DFT) [2] calculations including dispersion corrections [3]. The stability of all M@AlN monolayers, NO adsorption configurations, electrochemical pathways involving proton-electron pair ($H^+ + e^-$) transfer, and the corresponding free energies (using computational hydrogen electrode (CHE) approximation)[4] are computed. Among our modelled SACs, Pd@AlN is found to be the most promising one, which efficiently converts adsorbed NO molecule to NH_3 with a lowest limiting potential of -0.22 V. Further, it significantly suppresses the main competitive hydrogen evolution reaction (HER), resulting in high Faradaic efficiency for NH_3 production. This work may shed light on the design and exploration of new catalysts for NO reduction to NH_3 and provide a valuable reference for further experimental analysis.

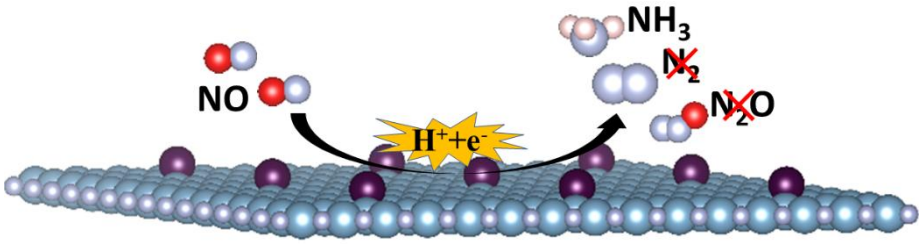


Figure 1: Sustainable development for the green environment - electrochemical conversion of toxic NO pollutant to value-added NH_3 through single-atom catalyst strategy

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Theoretical Chemistry Symposium
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State-to-State Transport Analysis: Unraveling Quantum Pathways in Molecular Aggregates

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Transport in molecular aggregates—whether of excitations, charges, or other quantum particles—can proceed along multiple competing pathways, each shaped by distinct pumps, drains and transport efficiency moderated by the thermal environment. While on-site populations might give an inkling of the pathway, in most real-world transport systems like photosynthetic light harvesting complexes and molecular wires, it is insufficient and lacks mathematical rigour.

We present the recently developed **state-to-state transport analysis**[1], which decomposes system dynamics into direct, time-resolved, unmediated flows between pairs of sites while fully incorporating environmental effects. This framework enables the reconstruction of transport pathways from the pairwise flows. A **non-Hermitian extension**[2] of this method can account for multiple sinks, yielding sink-resolved transport efficiencies while a more recent **Lindblad state-to-state formulation**[3] expands the scope further, incorporating pumps, dephasing, and arbitrary processes described by Lindblad operators.

We demonstrate these methods on excitonic and polaritonic systems, both with and without external pumps and drains. Importantly, our framework is simulation-agnostic, compatible with semiclassical, perturbative, and numerically exact techniques. Altogether, state-to-state analysis offers a rigorous and intuitive means of uncovering transport mechanisms in complex quantum systems, with direct implications for the design of materials optimized for quantum transport.

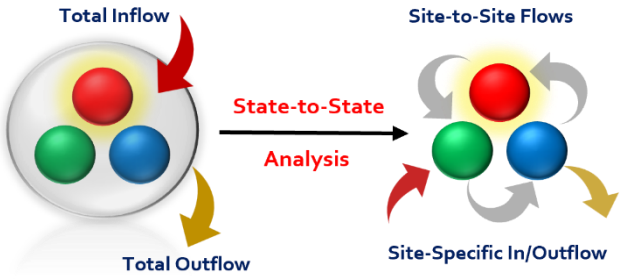


Figure A schematic describing State-to-State Transport Analysis

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Theoretical Elucidation of Photoelectron Spectrum of Diphosphatriazolate Anion, $P_2N_3^-$

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In this study, the 193 nm photoelectron spectrum of P_2N_3 is analyzed using comprehensive *ab initio* electronic structure and quantum dynamics computations, with a focus on the first five low-lying electronic states (X, $\tilde{A}$, $\tilde{B}$, $\tilde{C}$, and $\tilde{D}$) of P_2N_3. A 5 × 5 model Hamiltonian is constructed within a diabatic electronic framework to facilitate time-dependent (TD) and time-independent (TI) quantum chemical calculations. Nonadiabatic effects arise from energetically close electronic states possessing multiple crossings and conical intersections within them. The experimental photoelectron spectrum is thoroughly interpreted, accounting for all of the observed peaks and proper vibronic assignments. Notably, the first peak corresponds to four electronic states X, $\tilde{A}$, $\tilde{B}$ and $\tilde{C}$, while the second peak is attributed to the $\tilde{D}$ state of P_2N_3. Overall, our theoretical model deduced spectra coincide satisfactorily with the experimental results.

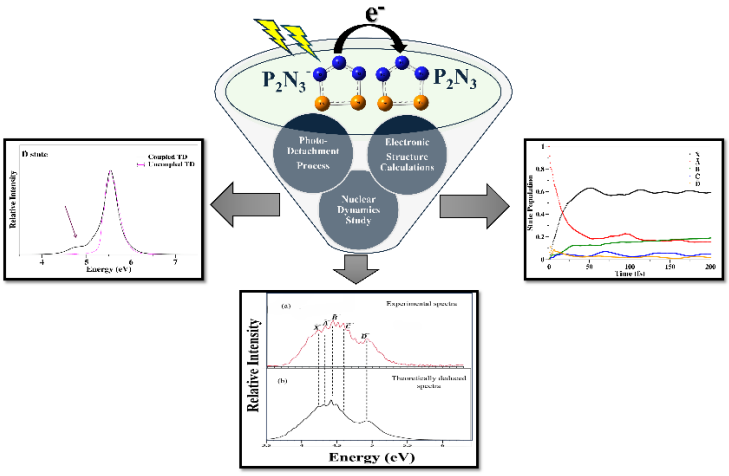


Figure 1 Pictorial diagramme of rationalizing exprimenal photoelectron spectra of P_2N_3 using vibronic coupling theory.

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Graph Neural Network–Driven Yield Prediction in Transition Metal–Catalyzed Cross-Coupling Reactions

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Machine learning (ML) is transforming diverse scientific disciplines, including chemistry. Among various ML approaches, graph neural networks (GNNs) have emerged as powerful frameworks for modeling complex relationships by representing data as graphs. One rapidly growing application of GNNs is in predicting chemical reaction yields. However, effectively managing heterogeneous datasets remains a significant challenge. In this study, we employed diverse datasets encompassing a range of transition metal-catalyzed cross-coupling reactions, including Suzuki, Sonogashira, Cadiot–Chodkiewicz, Ullmann-type, and Buchwald–Hartwig couplings. To predict reaction yields, we implemented and compared multiple GNN architectures—message passing neural networks (MPNN), residual graph convolutional networks (ResGCN), graph sample and aggregate (GraphSAGE), graph attention networks (GAT and GATv2), graph convolutional networks (GCN), and graph isomorphism networks (GIN). Among these, the MPNN model achieved the best performance, attaining an R^2 value of 0.75. When used for test data containing 90% Pd catalysts, the MPNN model achieved a predictive accuracy with an R^2 of 0.98 in chemical yield prediction. reactions. This work contributes to the application of machine learning in catalysis, providing valuable insights for optimizing catalytic reactions and contributing to innovations in sustainable chemistry and organic synthesis.

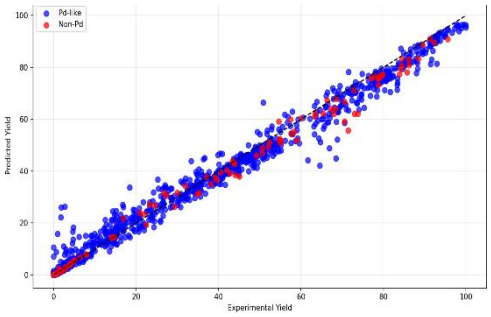


Figure3 : Scatter plots illustrating the performance of GNN models when tested for a dataset comprising 90% Pd catalysts

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Theoretical modelling of strongly correlated excited states of INVEST OLED molecules

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The unexpected violation of Hund's rule in certain N-heterocyclic chromophores, such as cyclazine and its derivatives, is often linked to an intriguing inversion of their low-lying excited singlet (S_1) and triplet (T_1) states [1,2]. This anomalous behavior, characterized by a negative singlet-triplet energy gap ($\Delta E_{ST} = E(S_1) - E(T_1)$), positions these molecules as promising candidates for next-generation OLED materials. Specifically, they serve as templates for fifth-generation OLEDs, leveraging reverse intersystem crossing (RISC) to enhance quantum yield via thermally activated delayed fluorescence (TADF). These so-called INVEST systems exhibit a delicate interplay of static and dynamic electron correlation, rendering them particularly challenging for conventional excited-state methodologies. Standard approaches such as CIS, RPA, and LR-TDDFT fail to accurately capture the singlet-triplet inversion, largely due to the inadequate treatment of double excitations in S_1 [1]. However, the intricate electronic structure of these systems—where S_0, S_1, and T_1 all involve significant contributions from double and higher-order excitations—necessitates a fine balance between static and dynamic correlation for reliable energy predictions. In this work, we undertake a comprehensive investigation of these molecules using a systematically layered hierarchy of single- and multi-reference wavefunction-based methods, alongside density functional theory (DFT) approaches. Our study is driven by three key objectives: (a) unraveling the essential electronic configurations that define the nature of the relevant states, (b) establishing high-fidelity benchmark data for excitation energies, and (c) identifying an efficient yet accurate computational protocol suitable for large-scale screening of more complex derivatives and oligomers. The ultimate goal is to pinpoint practical molecular candidates that exhibit optimal spin-orbit and spin-vibronic interactions, along with favorable ISC and RISC rate constants, for OLED applications. Furthermore, we examine the influence of spin contamination and spin polarization, drawing meaningful connections to minimal two- and three-state exciton models to distill the fundamental physics governing these exotic electronic interactions.



Figure 1: Violation Of Hund's law

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Theoretical Chemistry Symposium
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Exploring the magnetic behavior of {Ln2} Single Molecule Magnets with diverse bridging ligands. Synthesis and theoretical Insights.

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The magnetic properties of dinuclear lanthanide complexes arise from interactions between the two metal centers, often leading to cooperative effects that define their single-molecule magnet (SMM) behavior. Among the various factors influencing their energy barriers, magnetic exchange interactions are most significant.[1] The dimer geometry—particularly the spatial arrangement of the metal centers and the nature of the bridging ligands—strongly affects the overall magnetic response.[2] In this work, eight dihalide-bridged Dysprosium(III) complexes with F–, Cl–, Br–, and I– bridges, known for their large energy barriers, were selected for ab initio investigation. To further elucidate the role of di-μ-halide bridges and the co-ligands/terminal ligands, twelve additional model structures were generated by systematically substituting the halide ions within the parent complexes. These computational studies aim to rationalize how the donor strength and nature of the halide bridges modulate the magnetic exchange interactions and anisotropy in dinuclear Dy(III) systems. Additionally, we successfully synthesized a series of paddle-wheel-type {Ln_2} complexes (Ln = Tb, Dy, Ho, and Er), in which carboxylate bridges facilitate magnetic exchange. The nature of these interactions influences the overall magnetic properties.

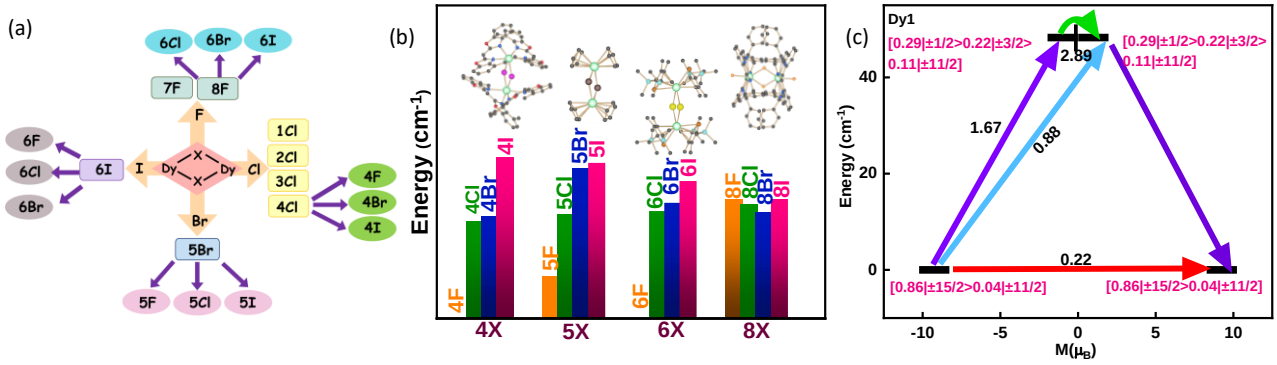


Figure 1 (a) Schematic representation of the design of model complexes from the parent complexes, and their comparitive energy barriers (b). (c) Energy barrier diagram of {Dy_2}.

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Theoretical Chemistry Symposium
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Tuning Hot Carrier Dynamics in Vacancy-Ordered Halide Perovskites through Lattice Compression: Insight from ab Initio Quantum Dynamics and Machine Learning

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The efficient harvesting of hot carriers (HCs) from high-energy photons can significantly enhance the optoelectronic performances. However, ultrafast HC cooling through intraband transitions poses a significant challenge for extraction using traditional semiconductor absorbers. The stable and compressible vacancy-ordered halide perovskites with isolated octahedra exhibit discrete electronic states at the conduction band edge, indicating the possible slow cooling of hot electrons (HEs). Using state-of-the-art ab initio quantum dynamics simulations and unsupervised machine learning (ML), we investigate the effect of lattice stress on HE dynamics in vacancy-ordered Cs_2SnBr_6. The moderate stress enhances structural rigidity and weakens dynamic electron−phonon interactions at the conduction bands. Such modifications and the widened energy gap at the conduction band edge partially suppress intraband nonadiabatic transitions, eventually elongating the HE lifetime. The pairwise mutual information extracts hard-to-find highly nonlinear dynamic structure-excited state property correlations, offering the unique opportunity to design efficient lead-free halide perovskites for HE-based optoelectronics strategically.

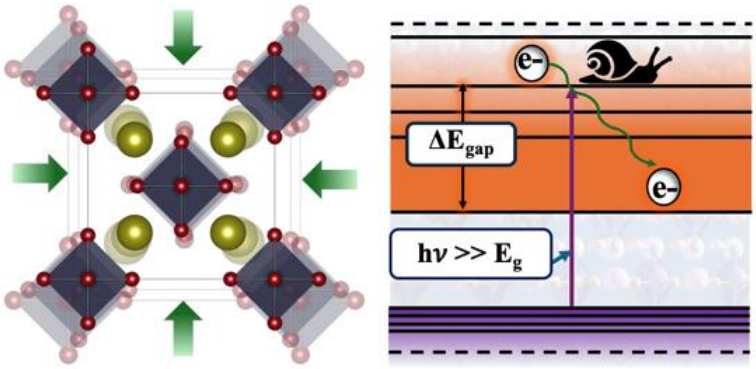


Figure 1: Hot carrier cooling in Vacancy-Ordered halide perovskite through lattice compression.

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Theoretical Chemistry Symposium
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Unraveling the Regioselective Reaction Mechanism of Gentisic Acid Catalyzed by SDO Enzyme

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Salicylate 1,2-dioxygenase (SDO), a ring-fission non-heme dioxygenase enzyme, displays a unique regioselective reaction with gentisic acid (GTQ) in the presence of molecular oxygen. Classical molecular dynamics simulations were carried out for both the wild-type SDO and its mutated variants, Asp174Glu and Asp174Ala, revealing the presence of three active water molecules at the enzyme's active site, pivotal in facilitating the oxidative cleavage of an aromatic C–C bond in the GTQ substrate [1]. Additionally, employing quantum mechanics/molecular mechanics (QM/MM) calculations, we unveiled three distinct reaction mechanisms explaining the regioselective oxidation of GTQ by the SDO enzyme. The formation of the main product, maleylpyruvate, via pathway A emerged as the most favorable mechanism, with a rate-determining barrier of 21.4 kcal mol^{-1}. Our study underscores the essential role of active water molecules in stabilizing the O_2 molecule and aiding in O–O and C–C bond cleavage, while also highlighting the crucial anchoring function of Asp174 in the enzymatic cycle. Moreover, upon introducing the G106A mutation to the wild-type enzyme, a significant change in catalytic activity was observed with two different substrates, salicylate and GTQ, attributable to the presence of a hydrogen bond network with water and the 5'-OH group of GTQ, which is absent in salicylate [2]. Long-range classical molecular dynamics simulations of both the wild-type SDO and its G106A mutant variant, each complexed with two different substrates, confirmed the existence of an inter molecular hydrogen bond network which is aligned with previous findings.

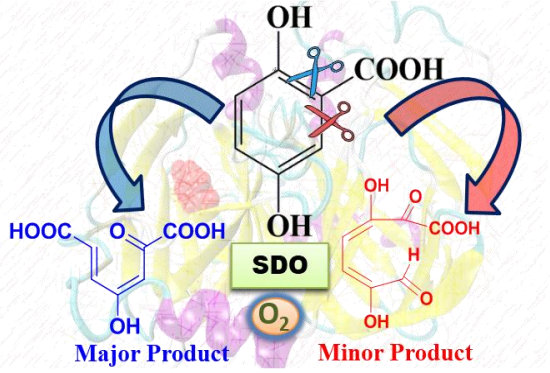


Figure 1 Dioxygenase activity of SDO on substrate GTQ.

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Theoretical Chemistry Symposium
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Molecular Mechanism of Stilbenoids Disruption Potential on Aβ42 Protofibril

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Amyloid-β42 (Aβ42) aggregation into protofibrils drives Alzheimer's disease (AD) pathology, making their disruption a key therapeutic strategy. We investigated five biphenolic stilbenoids—Resveratrol, Piceid, Astringin, Piceatannol, and Rhapontigenin—using docking, 500 ns molecular dynamics, MM-PBSA, and structural analyses (RMSD, RMSF, Rg, hydrogen-bond/salt-bridge dynamics, intersheet contacts, and PCA). All ligands bound β-sheet hotspots (Phe19, Phe20, Val36, Gly38). Rhapontigenin was most potent (ΔGbfe = −16.7 ± 5.8 kcal/mol), disrupting hydrogen bonds, salt bridges, compactness, and inducing chain-terminal deformation and conformational broadening. Piceatannol and Piceid showed moderate effects, while Astringin and Resveratrol were weaker. Rhapontigenin emerges as a strong scaffold for anti-amyloid therapeutics.

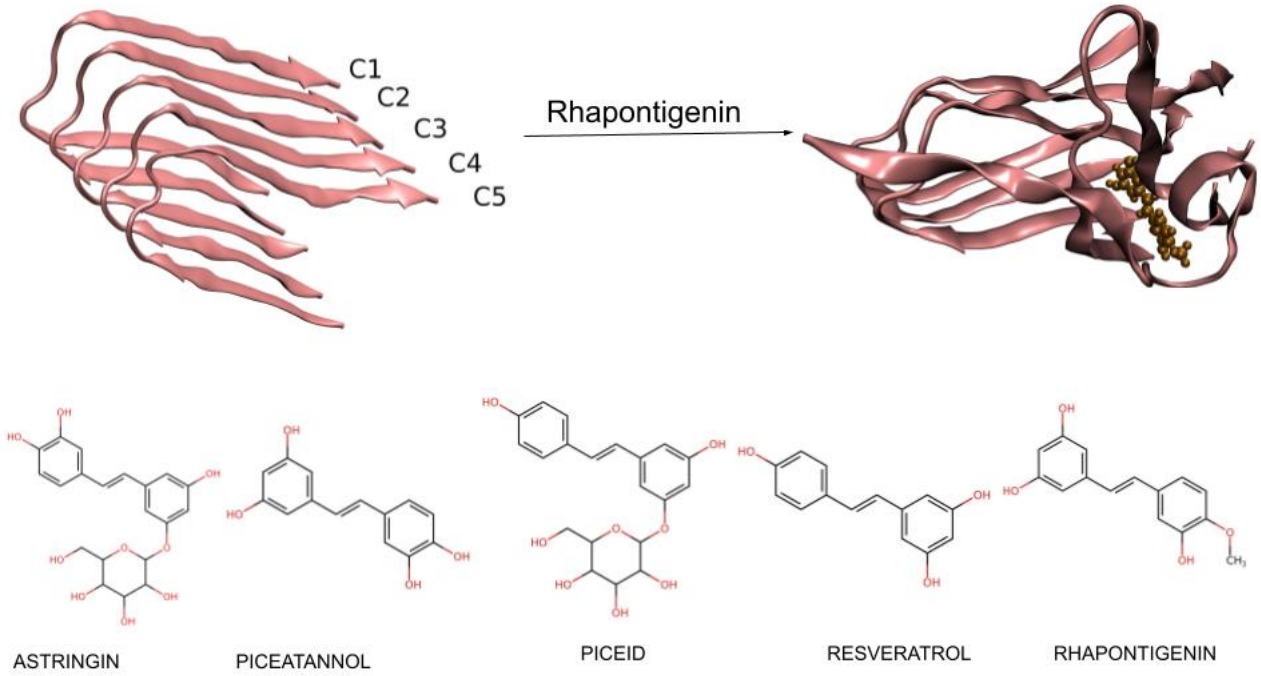


Figure: Snapshots of the configuration correspond to Aβ42 - Protofibril (2BEG) in the presence of Rhapontigenin at the beginning and at the end of the 600ns simulation. Thechemical structure of Astringin, Piceatannol, Piceid and Resveratrol are also incorporated. .

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Computational Study of effect of progressive p-Sulfonation at upper rim of Calix[4]arene on adsorption with small gaseous molecule.

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Complexation property of calixarene with various charged ions, drugs and neutral gaseous molecules is an old-age concept. Here, in present work we are performing theoretical calculations to understand the complexation of CO_2 molecule with biologically important supramolecule i.e. p-sulfonatocalix[4]arene (SC4A). We have performed a comparative study to check the stability of guest small molecule in unsubstituted calix[4]arene (C4A) and simultaneously with various sulfonatocalix[4]arene (SC4A) receptors. Also discussed how solvent environment specifically polar solvent affect the inclusion of guest molecule. Theoritical calculations like equilibrium geometry optimization, vibrational spectroscopy, global reactivity descriptors, themodynamic quantities and adsorption energy calculations led us to the result that HOMO-LUMO gap increases upon complexation of CO_2 with chosen receptor, adsorption energy of guest CO_2 molecule i.e., stability increases with progressive sulfonation[1].

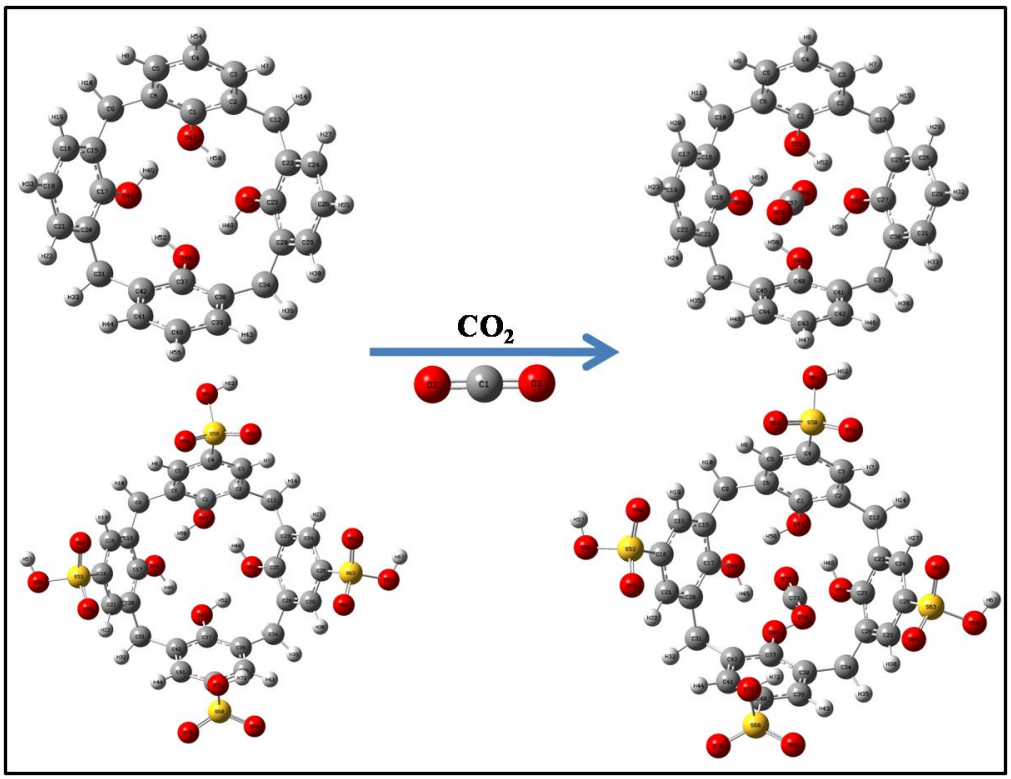


Figure 1: Inclusion of gaseous CO_2 molecule with chosen receptor molecules.

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Theoretical Chemistry Symposium
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Exploring Metal Nanoparticles to Degrade Per- and Polyfluoroalkyl Substances

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Abstract

Per- and polyfluoroalkyl substances (PFAS) are synthetic chemicals widely used in industrial and consumer products owing to their exceptional thermal stability and unique oil- and water-repellent properties.[1-2] However, they are extremely persistent and toxic to all forms of life, including humans. The strong C–F bonds in PFAS make their degradation challenging, necessitating the search for innovative solutions. Plasmonic metallic nanoclusters (NCs) are promising in efficiently converting sunlight into chemical energy, potentially driving the chemical reactions that are otherwise impossible (i.e., thermodynamically unfavorable) under standard conditions.

Bimetallic NCs of plasmonic and catalytic metals hold great potential for improving and controlling plasmon-induced hot-carrier generation, which is valuable in plasmonic catalysis.[3-4] In this study, we use first-principles real-time time-dependent density functional theory (RT-TDDFT) to explore hot-carrier generation in noble metal NCs (Ag, Au, and Cu) with site-specific doping by both noble and catalytic metal atoms (Ag, Au, Cu, Pd, and Pt). We find that the overall plasmonic response of the nanoparticle remains largely dependent on the surface atoms. At the same time, the generation of HCs and subsequent transfer to the PFAS molecules are strongly influenced by the dopant atoms. Doping with catalytic metal atoms (Pd and Pt) significantly enhanced the DHET from NC to PFAS. This suggests a promising route to tailor plasmon formation, its decay into HCs, and transfer to PFAS, thereby achieving complete degradation by selecting appropriate dopants.

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Theoretical Chemistry Symposium
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Second-Order Saddle Points and Concerted Reaction Mechanism: Insights from Entangled Trajectory Molecular Dynamics

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Reactions involving complex networks of transition states—such as those featuring bifurcations or higher-order saddles—require a molecular dynamics framework for accurate mechanistic insight. Quantum effects are crucial in certain regimes, but accounting for them remains challenging, especially for high-dimensional complex systems. A promising method in this context is the entangled trajectory molecular dynamics (ETMD) technique by Martens and coworkers[1], which employs quantum trajectories in phase space using Wigner distribution.

In this work, we apply ETMD to a two-degree-of-freedom Hamiltonian model[2] of double proton transfer, characterized by four minima, four rank-one saddles, and a rank-two saddle—providing a rich topological framework for mechanistic analysis. Guided by studies on higher-order saddles[3], we use Houk's delay time concept[4] to compare classical and quantum pathways and identify concerted dynamics. We observe significant fluctuations in the fraction of concerted trajectories even at energies above the second-order saddle. Notably, ETMD identifies energy regimes where classical trajectories become dynamically trapped, while quantum trajectories exhibit barrier-crossing behavior indicative of dynamical tunneling. These quantum pathways are further analyzed using Lagrangian descriptors[5] and entanglement entropy[6], offering a phase-space interpretation of quantum-enhanced concertedness.

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Computational analysis of inhibitors of Methionyl-tRNA synthetase in *Mycobacterium tuberculosis*

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Mycobacterium tuberculosis (*Mtb*) causes infectious disease tuberculosis (TB) which kills millions of people throughout the world.[1] Methionyl-tRNA synthetase (MetRS) is an enzyme that catalyzes the charging of tRNA with its cognate methionine. Disturbance in the enzymatic activity of MetRS will accumulate uncharged tRNA and disturb protein synthesis. MetRS from *Mtb* shares low sequence and structural similarity with human MetRS, making it a promising target. There are several inhibitors reported for *Mtb* MetRS. We docked the selected 82 inhibitors with known experimental inhibition activity at the active site of *Mtb* MetRS.[2,3] Four different docking algorithms were used to remove noise. These inhibitors act as dual-site inhibitors by occupying either two site (methionine, ATP, and tRNA acceptor arm site) and interact with the catalytic domain, connecting polypeptide (CP) domain, and KMSKS domain (**Figure 1**). One of the docked inhibitor-bound MetRS was subjected to molecular dynamics (MD) simulation, and the results indicate the stability of the inhibitor (inhibitor RMSD with respect to protein 0.67 nm) within the binding site of MetRS throughout the simulation.

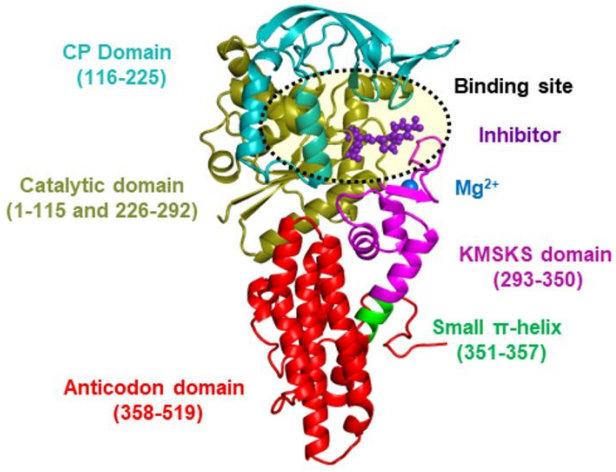


Figure 1 Structure of *Mtb* MetRS with docked inhibitor.

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Hydrophobicity and Concentration Governing the Role of Amino Acids in Methane Hydrate Nucleation

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In the present work, nanoscale molecular dynamics simulations are performed to investigate nucleation and growth of methane hydrates in the presence of amino acids of different hydrophobicity (valine, serine, and asparagine) over a concentration range of 0 to ~3 wt%. The results showed that both the type and concentration of amino acids affect the hydrate formation. At low concentrations, valine and serine promoted hydrate formation, whereas at higher concentrations, they act as inhibitors. In contrast, asparagine did not promote hydrate formation at any concentrations, restricting methane encapsulation to below 18%. Interaction energy analysis revealed that van der Waals interactions govern nucleation, with valine exhibiting the strongest contribution. Hydrogen bonding analysis showed that each molecule of valine, serine, and asparagine forms approximately 5, 6, and 8 hydrogen bonds, respectively, with water molecules. The effect of side chain is found to be negligible for valine, however, significant for asparagine. At higher concentrations, enhanced amino acid–water interactions disrupted the structural ordering of water molecules. The obtained F4 values confirmed the coexistence of hydrate cages with disordered water networks. The radial distribution functions further supported methane dispersion and subsequent encapsulation.

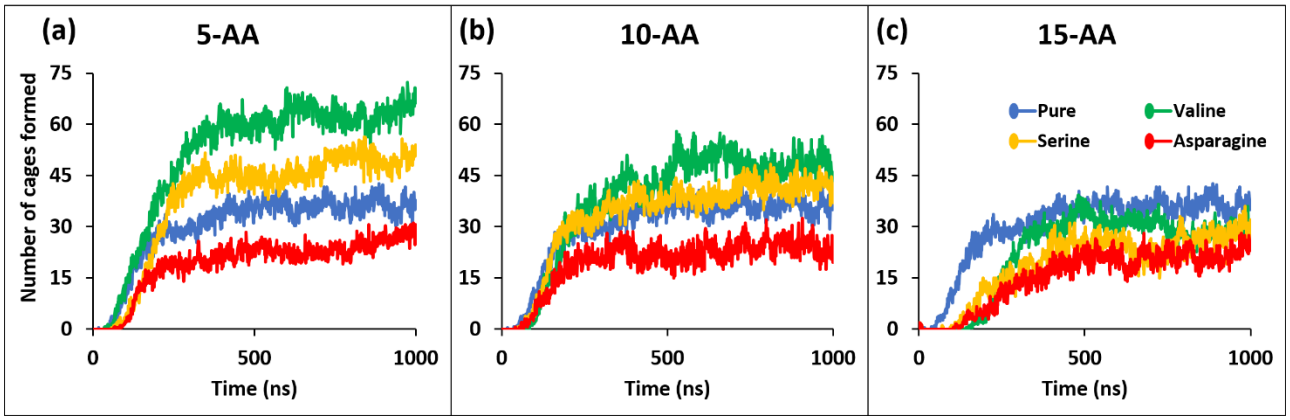


Figure: The average number of cages formed during simulations in the presence (a) five molecules (b) ten molecules (c) fifteen molecules of various amino acids.

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MD-guided design of hybrid polymer-protein conjugates with tuneable aqueous solubility

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Polyethylene glycol (PEG) is a hydrophilic polymer well known for its minimal protein and cell adsorption, making it one of the most biocompatible materials available. It is highly soluble in water, ethanol, and various organic solvents at ambient conditions, and exhibits excellent lubricity, moisture retention, and non-toxic, non-immunogenic behavior. However, PEG alone lacks functional groups necessary for bio-interactions and network formation, limiting its direct use in injectable formulations. To overcome this limitation, PEG is often conjugated with biocompatible and biodegradable polymers to form amphiphilic block copolymers with tunable physical and chemical properties.

Among these, poly(L-lysine) (PLL) is a cationic, biodegradable polypeptide known for its ability to interact electrostatically with negatively charged biomolecules, including proteins and nucleic acids. Recent studies have demonstrated that PEG_m–PLL_n and PEG_m–PLL_n–PEG_m copolymers can self-assemble into nanostructures or form injectable hydrogels suitable for biomedical applications such as tissue regeneration, gene delivery, and localized drug release.

In this study, we focus on the rational design of PEG–PLL-based amphiphilic block copolymers—specifically PEG_m–PLL_n and PEG_m–PLL_n–PEG_m architectures—to explore their potential in forming polymer–protein hybrid systems. The incorporation of the PLL block provides tunable charge density and hydrophilicity, enabling modulation of PEG's solubility, structural conformation, and protein interaction behavior in aqueous environments.

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Computational Insights into FeCO and FeC_2O Molecules of Interstellar Interest

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Iron in its elemental state is rarely encountered in the interstellar medium despite being the most prevalent refractory element. The recent detection of the FeC radical within the envelope of IRC+10216, along with the probable existence of iron oxide in the interstellar medium, suggests the feasibility of identifying iron-carbon-oxygen systems, thus explaining the limited observation of iron compounds. In light of this potentiality, the potential energy surface of FeC_2O in its neutral state has been computationally analyzed using four distinct levels of theory, leading to the identification of twenty, six and ten isomers in the singlet, triplet and quintet electronic states respectively. The triplet and quintet electronic states of the isomers of FeC_2O have also been explored using the UωB97XD/6–311++G(2d,2p) level of theory. The global minimum for FeC_2O is a linear structure at the quintet electronic state. Various computational tools, including AdNDP, FMO analyses WBI, NBO, ELF, and AIM, have been employed to understand the bonding characteristics of the global minimum geometry. The *ab initio* molecular dynamics (AIMD) simulations confirm the kinetic stability of the global minimum geometry. The IR and microwave spectroscopic parameters have also been obtained at the ωB97XD/6–311++G(2d,2p) level of theory. The total and partial density of states have been plotted to examine the contributions of various atoms to the electronic structure. The structural, energetic, and spectroscopic parameters depicted in this study hold significant implications for prospective astronomical investigations.



Figure 1: . Ground state geometry of FeC_2O obtained at the UωB97XD/6-311++G(2d,2p) theoretical level**.**

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In Silico Studies Demonstrate that −OBO Units Bound to Stable Boron Cages in $YB_{11}(OBO)_{12}^-$ (Y=C/Si) Anions Provide a Desirable Borate-Rich Solid Electrolyte Interface in Calcium-Ion Batteries

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Calcium-ion batteries (CIBs) have emerged as promising energy storage devices, offering higher volumetric capacities and lower redox potential (−2.87 V vs SHE). However, the development of efficient electrolytes for CIBs remains a bottleneck due to the formation of Ca^{2+}-impermeable passivation layers on the Ca anode. Hence, there is an urgent need to develop electrolytes that form Ca^{2+}-permeable solid electrolyte interfaces. Herein, calcium salts of $YB_{11}X_{12}^-$ (Y = C/Si and X = −BO/OBO) anions were investigated using density functional theory (DFT)-based simulations for application in CIBs.[1] DFT computations revealed the oxidative stability of these anions, while *ab initio* molecular dynamics (AIMD) simulations unraveled their reductive behavior over the Ca surface. The vertical detachment energies, frontier molecular orbital analyses, and oxidation-reduction potentials were systematically probed. Time-dependent charge transfer and projected density of states were analyzed to gain atomistic insights into the electrolyte-anode interface. Our simulations reveal that $YB_{11}(OBO)_{12}^-$ (Y = C/Si) anions decompose over the Ca anode in such a way that the borane cluster remains stable while the –OBO ligands transform to give borate species in the solid electrolyte interface. Notably, borates have been reported in the literature to allow for the reversible plating/stripping of calcium.[2] Hence, this computational study predicts that $Ca[YB_{11}(OBO)_{12}]_2$ (Y = C/Si) can be a promising CIB electrolyte. All in all, our work introduces a fresh perspective for developing suitable CIB electrolytes, going beyond ensuring the stability of the electrolyte on the anode.

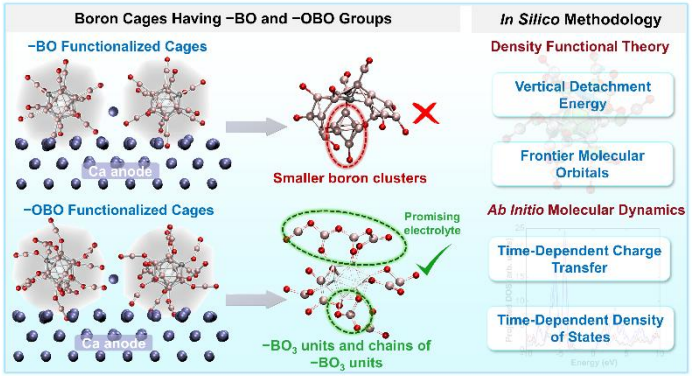


Figure 1 Graphical overview illustrating the central idea and methodology of the study.

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Accelerated Hydrogen Atom Transfer in aqueous medium by Mn(V)-oxo non-heme complex and BNAH

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Water serves as a reaction medium in enzymatic redox catalysis, dictating reaction rates, selectivity and atom transfer[1] by forming hydrogen bonds[2] and generating electric field gradients[3]. These properties tune the redox potentials of metal-centred enzymes, stabilising charged intermediates and facilitating electron transfer. Fe-bTAML non-heme complexes designed to mimic cytochrome P450 enzyme[4] show that Fe(V)-oxo intermediates react faster in water than in acetonitrile, but are too unstable for detailed experimental study. This limitation redirects the study to Mn(V)-oxo intermediates[5], which exhibit even higher reactivity and stability in water. Theoretical calculations indicate a spin crossover, where triplet states drop below singlet states as the reaction progresses. Analysis of minimum energy crossing points (MECPs) reveals significant charge transfer from BNAH to the metal complex, where the polarity of water and hydrogen bonding dramatically enhances the rate and reactivity. Further understanding of solvent ratio-dependent rate acceleration is still in progress.

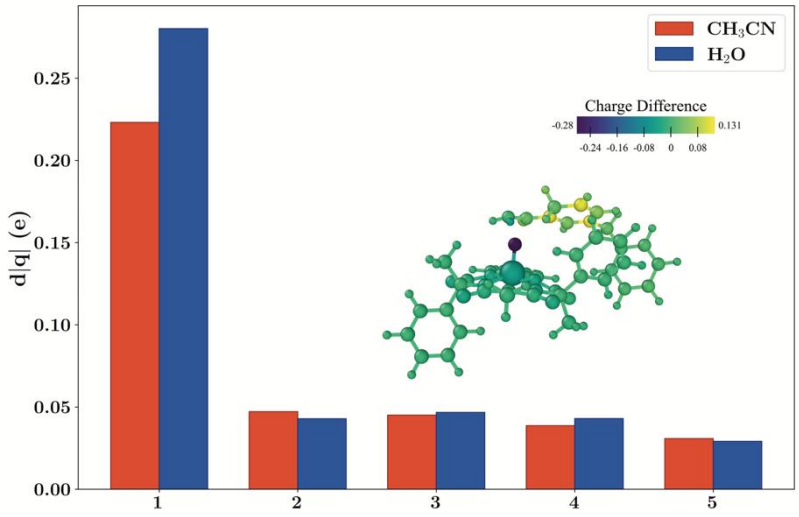


Figure 1: Difference in partial charges on atoms (major contributors) between MECP and ground state

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Prolate–Oblate Control of Toroidal States in 3d–4f Rings

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Single-molecule toroics (SMTs) are molecular systems in which local anisotropy axes of lanthanide ions arrange in a circulating fashion around a cluster, producing vortex-like toroidal moments.SMTs are of great interest due to their potential applications in quantum computers, spintronics, and magnetoelectric devices.[1] Since the first observations of SMT behavior in Dy3 molecules[2], efforts have been made to extend the phenomenon to larger and more complex topologies. Herein, we present four heterometallic 3d-4f molecular wheels, $[Mn_8^{III}Ln_8^{III}(mdea)_{16}(L)_8(NO)_8]$ (Ln = Dy,Ho,Er,Yb, L = benzoate/ortho-toluate respectively).[3] *Ab initio* calculations on $[Ho_8Mn_8]$, $[Dy_8Mn_8]$, $[Er_8Mn_8]$, and $[Yb_8Mn_8]$ using MOLCAS 8.2 show an unexpected reversal in toroidal behavior. CASSCF/SINGLE_ANISO provides the orientations of the local anisotropy axes, which POLY_ANISO subsequently maps into exchange-coupled state diagrams. Surprisingly, our $[Ln_8Mn_8]$ clusters show the opposite trend. Prolate Er^{3+} and Yb^{3+} ions stabilize clear toroidal ground states. This unexpected behavior shows that even small changes in cluster structure and exchange pathways can override the usual oblate–prolate rules, offering new insight into how toroidal states can be controlled at the microscopic level in lanthanide–transition-metal clusters.

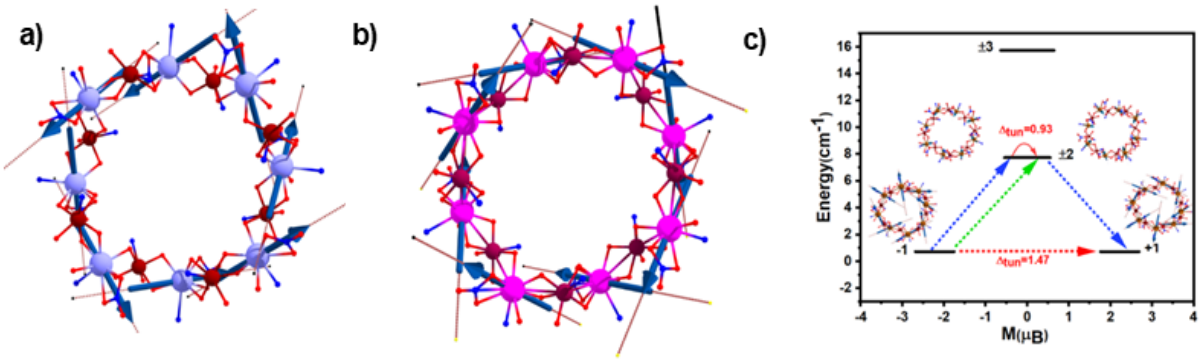


Figure 1 : a) and b) The directions of the local anisotropy axes in the ground doublets on the Ln sites, i.e, **Er^{3+}** and **Yb^{3+}**, respectively. **c)** Low-lying exchange spectrum in **Ho^{3+}**.The exchange states are placed on the diagram per their magnetic moments (bold black lines). The red arrows show the tunnelling transitions (energy splitting) within each doublet state, while the green/blue arrows show the possible pathway through Orbach/Raman relaxation.

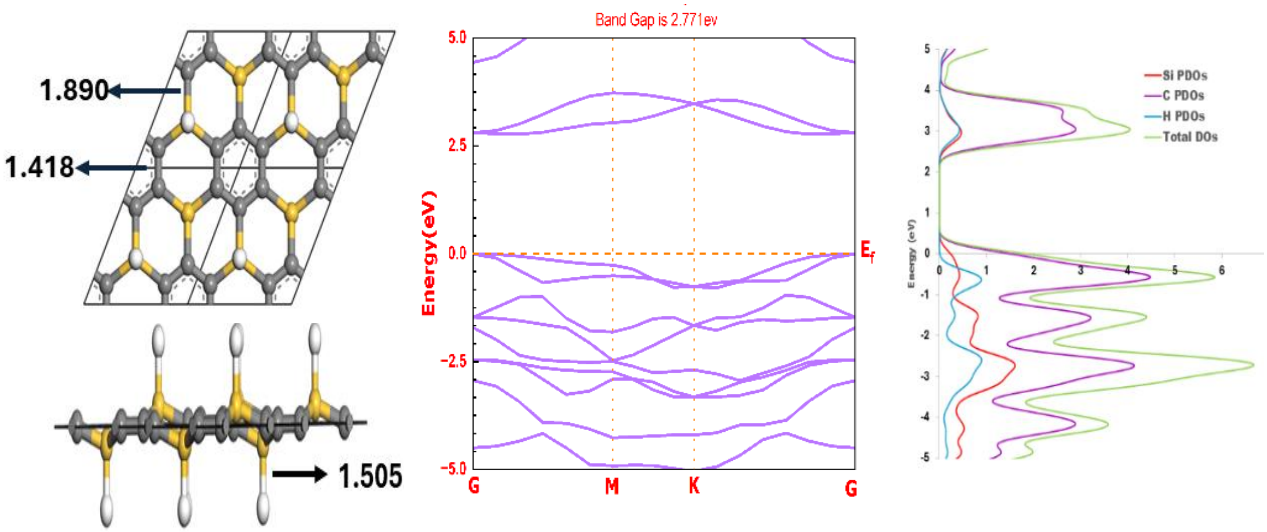
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Band-gap Engineering in graphene by Sextet Localization: XSiC3

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The main disadvantage of the wonder material graphene is the absence of band gap due to its high hexagonal *P6mm* symmetry. From the perspective of Clar's aromatic sextet theory[1], this degeneracy is associated with three-fold degeneracy of its Clar structure. This degeneracy must be destroyed to localize the sextets and open the band gap. Introducing sp^3 hybridized atoms as defects in conjugation allows localization of the sextets. Preserving the high hexagonal symmetry demands 1:3 stoichiometry of sp^3 and sp^2 atoms (z=8). Silicon is an ideal choice for sp^3 defect as it ensures minimal perturbation of the aromatic sextet and also assures a strong σ-framework, as silicon prefers single bonds. Our DFT calculations (CGA-PBE with plane wave cutoff 450eV) on HSiC3, which is isostructural to the SiC3(*P6/mmm*)[2] theoretically reported earlier to have a zero-bandgap, indeed open a semiconducting gap due to the promotion of silicon hybridization to sp^3. The valence and conduction bands are doubly degenerate at Gamma and K and are dominated by unhybridized C-p_z orbitals mapping to the HOMO and LUMO of the aromatic sextet ring.



(a) **(b)** **(c)**

Figure 1 : (a) The unit-cell of SiC_3H 2D sheet. (b) Electronic Band Structure. (c) Atom projected DOS.

The existence of a direct band-gap and the flexibility of hosting a variety of functional groups on silicon and availability of rational synthesis as in the experimentally characterized NC3 [3] makes the 2D-materials an attractive target for a variety of applications that are impossible with graphene.

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Interfacial Behaviour of BMIMCl Ionic Liquid-Water Mixture With an Optimized Classical Forcefield for Water Activity

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Ionic liquids (ILs) are considered better alternatives to common surfactants and chemicals used in enhanced oil recovery (EOR), solvent extraction, and biomass conversion.[1] Molecular simulations help in designing ILs by giving a molecular-level understanding of these processes. However, force fields developed for bulk ionic liquids often face transferability problems in aqueous systems. Using osmometry, we earlier reported (Dhabal et al. *Phys. Chem. Chem. Phys*., 2020, **22**, 28325) a simple parameter modification of the widely used nonpolarizable OPLS-based force field for BMIMCl IL, making it suitable for use with the SPC/E water model.[2] The re-parameterized model reproduces the thermodynamic, dynamical, and structural properties of BMIMCl-water mixtures. In this work, we study the interfacial behaviour of BMIMCl-water mixtures using this re-parameterized force field and compare the critical micellization concentration (CMC) from different experiments for short-chained BMIMCl.[3] Our results show that the re-parameterized model reproduces experimental water activity and liquid–vapor interfacial tension across different compositions. Similar to experiments, the simulations show that interfacial tension measurements give higher CMC values than osmotic coefficient, conductivity, and viscosity measurements.[4] The study indicates that BMIMCl, due to its short alkyl chain, is less surface-active than common surfactants and first forms small aggregates in the bulk before significantly populating the interface. This is different from the typical micelle formation pathway of surfactants. Our study suggests that surface tension measurements may not be suitable for obtaining reliable CMC values for some short-chained ILs. The reparameterized force field developed here can be utilised to investigate the molecular-level mechanisms in solvent extraction and EOR applications.

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Quasi-Classical Trajectory Study of the CN^- + CH_3I Reaction on a High-Dimensional Neural Network PES

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The gas-phase dynamics of bimolecular nucleophilic substitution (S_N2) reactions have been extensively studied by both experimental and theoretical groups due to their broad applicability and the emergence of new mechanistic insights. The reaction between CN^- and CH_3I is particularly intriguing, as it can yield two isomeric products ($NCCH_3$ or $CNCH_3$ + I^-) owing to the ambident nature of the CN^- nucleophile. Previous velocity map imaging experiments revealed predominantly direct rebound dynamics and high internal energy excitation in the reaction products. In another study, direct dynamics simulations were performed employing PM7 semi-empirical method and B3LYP/aug-cc-pVDZ/ECP density functional theory (DFT); however, these approaches were limited by insufficient number of DFT trajectories (due to high computational costs) and an overestimation of hydrogen transfer reactions with PM7. In the present study, a high-dimensional neural network-based potential energy surface (PES) was developed using extensive electronic structure data. The PES was rigorously validated using established benchmarks and subsequently employed in quasi-classical trajectory simulations. A substantial number of reactive trajectories were generated, enabling a detailed analysis of the reaction dynamics. The simulation results are consistent with previous findings and provide new insights into the mechanistic pathways of this SN2 reaction.

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Electronic Structure Fingerprints of Proton-Coupled Electron Transfer in Iron–Oxo Complexes: Mapping Synchronous to Asynchronous Pathways

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Proton-coupled electron transfer (PCET) lies at the heart of biological energy transduction and synthetic catalysis, providing a fundamental bridge between proton and electron flow. Understanding how PCET operates—whether in synchronous or asynchronous regimes—is essential for unraveling complex reaction mechanisms. C–H oxidation offers an exemplary platform to probe these questions, where electronic structure features dictate whether hydrogen atom transfer (HAT) or PCET pathways dominate. High-valent iron–oxo complexes, long recognized as biomimetic analogues of enzymatic oxidants, provide a powerful testbed for discerning such mechanistic preferences.

Through DFT and multireference electronic structure analyses (CASSCF/NEVPT2) of biomimetic Fe–oxo inetrmediates, our investigations present that subtle changes in Fe–O bonding and spin-state energetics decisively tune the balance between HAT and asynchronous nature of PCET pathways. The emergence of oxyl character promotes HAT, while its attenuation favors PCET, with the mechanistic crossover governed by electronic configuration and geometric distortions of the Fe–oxo core. These insights reveal the electronic fingerprints that differentiate synchronous from asynchronous PCET, linking redox tuning of the metal–oxo unit to control over proton and electron transfer events.

By clarifying how electronic structure underscores HAT versus PCET reactivity, this work advances a general framework for interpreting PCET fingerprints in biomimetic iron–oxo complexes. More broadly, it highlights asynchronous PCET as a key concept for connecting geometric and electronic structure to oxidative reactivity, offering design principles that extend from synthetic complexes to enzymatic catalysis and mechanistic biology.

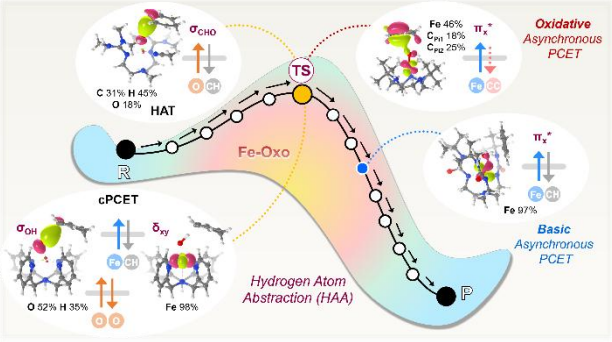


Figure 1 Reaction coordinate for C–H oxidation by Fe–oxo complexes, showing the HAT, concerted PCET, and asynchronous PCET pathways. Orbital and spin-state analyses highlight electronic fingerprints that distinguish oxidative and basic asynchronous PCET from conventional HAT.

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B−B Sites in Molten Boron Oxide are Superior to Cyclic B−O−B Sites for Methane Oxidation to Formaldehyde and Carbon Monoxide

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Boron oxide (B_2O_3) is a promising metal-free catalyst for the oxidative dehydrogenation (ODH) of methane, yielding high selectivity for formaldehyde (HCHO) and carbon monoxide (CO) at 823 K. Since the reaction occurs above the melting point of B_2O_3 (~725 K), it likely proceeds in the molten state. Building on our earlier work on methane ODH over crystalline boron oxide[1,2] and hexagonal boron-nitride[3]. Here, we present a detailed DFT-based mechanistic study of methane oxidation over these structural motifs with $^1O_2$ and $^3O_2$.[4] The results identify the B−B site as the most catalytically active motif for HCHO formation, requiring a low activation barrier of 36.6 kcal mol^{-1}. In contrast, cyclic B−O−B motifs exhibit substantially higher barriers (~50–78 kcal mol^{-1}). Orbital analyses highlight distinct electron transfer pathways: oxygen lone-pairs in B−O−B rings, versus σ(B−B) bond donation at B−B sites. Additionally, CO formation is predicted to be thermodynamically more favorable than CO_2, consistent with existing experimental trends.

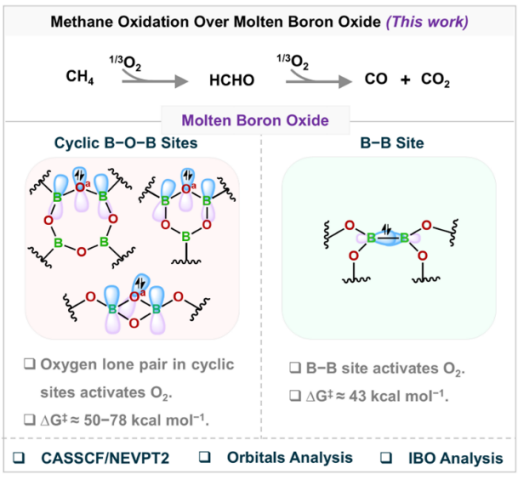


Figure 1 Oxidative Dehydrogenation of Methane over Molten Boron Oxide

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Theoretical Chemistry Symposium
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Redox-Switchable symmetry transition in Benzoquinone-Bridged Co(II) SMM: a DFT and Ab-initio ligand field study

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The development of high-performance single-molecule magnets (SMMs) benefits significantly from the metal-radical approach, which enables precise control over magnetic exchange interactions and molecular geometry. Here, we report two benzoquinones bridged dicobalt complexes $[\{Co^{II}(L\text{-}N_4)\}_2(\mu\text{-}X)](ClO_4)_2$ (X = CA^{2-}, **1**; X = BA^{2-}, **2**; L-N_4 = N,N'-bis((2-N-methylimidazol-1-yl)methylene))-2,2-dimethylpropane-1,3-diamine) and their reduced counterparts, $[\{Co^{II}(L\text{-}N_4)\}_2(\mu\text{-}X)](ClO_4)\cdot n$MeCN (X = $CA^{3-,\bullet}$, n = 5, **1R**; X = $BA^{3-,\bullet}$, n = 2, **2R**). In this work, we present a systematic computational investigation that combines Broken Symmetry Density Functional Theory (BS-DFT) and multireference CASSCF calculations to assess how incorporating radical bridges with a specific coordination environment affects the electronic structure, magnetic exchange coupling, and magnetic anisotropy in a system. Structural, magnetic measurement, and theoretical calculations reveal that **1** and **2** possess nearly perfect trigonal prismatic geometry, exhibiting remarkable axial magnetic anisotropy (D_{Co} = -108 to -114 cm^{-1}). In contrast, the reduced radical-bridged systems **1R** and **2R** undergo a geometric transition to octahedral coordination while retaining significant uniaxial magnetic anisotropy (D_{Co} = -37 to -52 cm^{-1}). magnetic investigations demonstrate strong antiferromagnetic interactions between Co(II) ions and bridging radicals (~-150 cm^{-1}) in **1R** and **2R** the largest reported for the metal-benzoquinone system. All complexes display single-molecule magnet behavior, with the systems (**1** and **2**) showing unique metamagnetic ordering and Raman relaxation processes induced by intermolecular π-π stacking interactions.

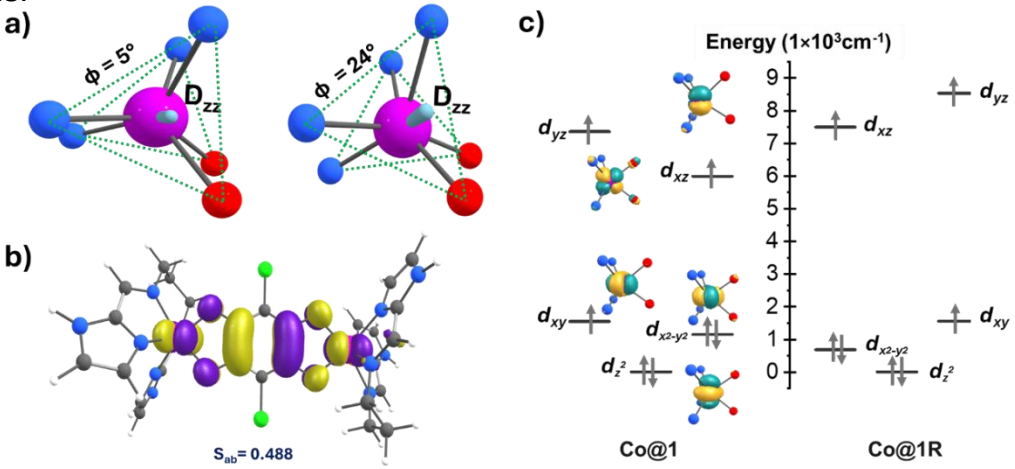


Figure 1 **(a)** NEVPT2 computed the orientation of the main anisotropic (D_{ZZ}) axes shown using the core of [CoN4O2] of **1**(left) and **1R**(right); **(b)** DFT computed overlap integrals responsible for the Co-radical coupling in 1R plotted with an isosurface value of 0.004 $e^-/bohr^3$. **(c)** Ab initio ligand field theory (AILFT) computed d-orbital ordering for Co@**1** (left) and Co@**1R** (right). Color code: Co (pink); N (blue), O (red), Cl(green), C (grey), and H (white).

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Modeling X-ray Emission Spectroscopy of Metal Complexes

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X-ray Spectroscopy is a powerful analytical technique used to study the composition, structure, and electronic state of materials. In particular, X-ray Emission Spectroscopy (XES) is a powerful technique that provides insights into the bonding nature, spin state, and the effects of oxidation state changes on the spectral features of metal complexes. However, XES is less utilized due to the need of advanced equipment like synchrotron radiation sources, limited accessibility, and safety issues. Linear response time-dependent density functional theory (LR-TDDFT) method[1] and the one-electron [2] approach are regularly used for computing the Vtc-XES spectra. In this project, we focus mainly on the Kβ ($3p \rightarrow 1s$) spectra of transition metal complexes and Lβ ($4d \rightarrow 2p_{3/2}$) Lanthanide complexes. While LR-TDDFT and one-electron approaches can accurately predict Vtc-XES when the ground electronic state can be represented well with a single Slater determinant. However, these methods struggle when ground state of a chemical system is multiconfigurational or when multiexcitonic states are involved in the excited states. To overcome these issues, we are also modeling XES with multiconfigurational methods such as Restricted Active Space Self-Consistent Field (RASSCF) and Restricted Active Space Second-Order Perturbation Theory (RASPT2) that helps to include the static and dynamic correlations to the calculation in an efficient way.

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Spatiotemporal Dynamics in Supramolecular Polymer

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Unlike covalent polymers, supramolecular self-assemblies are structures formed through weak, non-covalent interactions between constituent monomers. These interactions make the assemblies dynamic and reversible in nature. This allows the synthesis of many supramolecular polymers, often inspired by biological systems such as actin filaments and microtubules. The formation of these biological systems involve many kinetic mechanisms like nucleation, polymerization and depolymerization leading to complex temporal and spatial behaviour. Inspired by these biological examples, we aim to model and understand the dynamic (dis)assembly of synthetic supramolecular polymers. For this, we use a simplified version of coupled cooperative kinetic model that captures essential steps of supramolecular polymerization like (de)activation of monomers, nucleation, polymer elongation, and deactivation of polymer chain.[1] To analyze the model, we explore its parameter space by performing linear stability analysis around the steady state. This analysis reveals two distinct regions in the parameter space: one where the perturbation on the homogeneous steady state decays and the system returns to equilibrium, and another where the perturbation increases and the system becomes unstable. Numerical integration on the coupled ordinary differential equations (ODEs) reveal that the unstable region corresponds to the limit cycle, where oscillations in the monomer and polymer concentrations are possible. Along with temporal dynamics, we are interested in studying the spatial organization of supramolecular polymers. Hence, we extend the model using a continuum reaction-diffusion approach in two dimensions. Initial simulations within the limit cycle region on the 2D lattice reveal the emergence of wavefront-like structures that oscillate and propagate outward. We further intend to study and characterize these patterns formed as a function of the model parameters.

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Single-molecule magnetic and Single-molecule toroic behavior of 3d-4f complexes

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Single molecular magnets (SMMs) are molecules that show magnetic relaxation below their blocking temperature (T_B) in the absence of a magnetic field. SMMs are highly interesting due to their potential applications in memory storage devices, Quantum Bits, etc.[1] SMMs were primarily searched on the 3d or Lanthanide (Ln) based mononuclear and polynuclear complexes. Due to the combination of the large spin of 3d ions and the spin/anisotropy of lanthanide ions, heterometallic 3d/4f complexes have recently attracted much attention. Moreover, some polynuclear 4f/3d-4f systems exhibit Single-Molecule Toroids (SMTs) behaviour, which are bistable molecules similar to Single-Molecule Magnets (SMMs) but with a toroidal magnetic state. The noncollinear arrangement of the magnetic moments of each metal centre in SMTs can lead to interesting magnetic properties due to their high molecular symmetry.[2] Here, we discuss the magnetic behaviour of a series of $\{M^{II}_3Ln^{III}_3\}$ (M = Ni, Zn and Ln = Dy, Tb, Gd) complexes.[3] Ab initio and Density Functional Theory (DFT) calculations were performed using the MOLCAS 8.2 and GAUSSIAN 16 programs, respectively, and the calculations align with the experimental prediction. Structural parameters and computational studies for the $\{Co^{III}_4Ln^{III}_2\}$ (Ln = Tb, Dy, Ho) system will also be discussed.

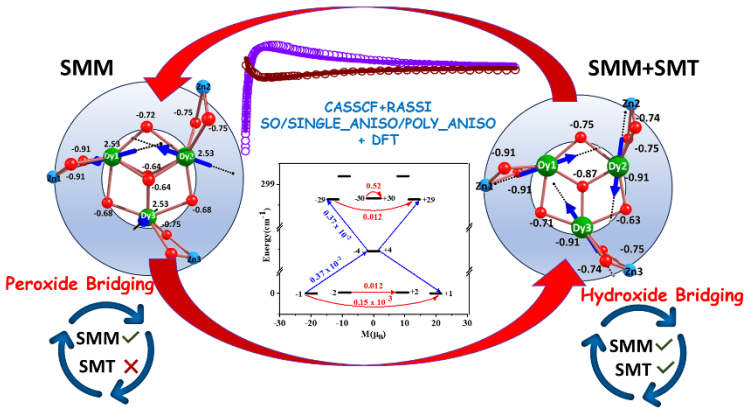


Figure 1. The role of bridging ligands in modulating 3d-4f SMM and SMT behaviour.

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Computational Insights into Homo-bimetallic Cooperativity for Photocatalytic CO_2 Reduction

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Photocatalytic conversion of CO_2 into value-added products offers a sustainable approach to reducing greenhouse gas emissions. Multinuclear metal catalysts typically show greater selectivity and activity than monometallic analogues due to synergistic interactions between metal centres. Homo-bimetallic copper complexes are especially effective in reducing CO_2 to carbon monoxide (CO), formate ($HCOO^-$) and hydrogen (H_2) through cooperative metal–metal interactions. Here, Density Functional Theory (DFT) calculations were used to investigate the mechanisms of $[(L)CuCu]^{2+}$ with $[Ru(phen)_3]^{2+}$ as photosensitizer and BIH/TEOA as a sacrificial donor under ambient conditions. Formation of $HCOO^-$ and H_2 proceeds via a metal hydride intermediate, supported by computed ^1H NMR chemical shifts. The minimum-energy pathway for CO formation involves C–O bond cleavage of a CO_2 molecule bridging between the two copper centres. Energy profiles highlight the role of Cu–Cu cooperativity and photosensitizer efficiency in directing selectivity between CO and $HCOO^-$ formation. These findings underscore the potential of homo-bimetallic copper photocatalysts for green hydrogen production and carbon recycling, advancing sustainable energy applications.

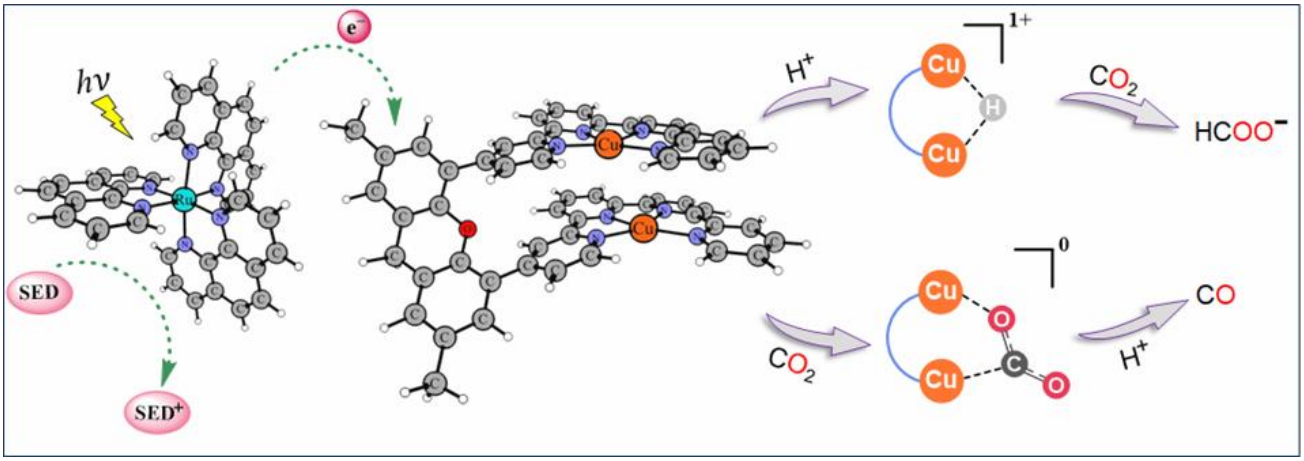


Figure 1. Schematic representation of proposed reaction mechanism for photocatalytic CO_2 reduction via homo-bimetallic cooperativity.

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Sequence, Structure, and Solvation Environment: Divergent Allosteric Pathways in Viral TAR RNA Recognition

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RNA recognition by viral proteins is not dictated by static structure alone but by hidden allosteric channels and solvent responses. Using atomistic simulations and free-energy methods, we compare TAR RNA from HIV-1, HIV-2, and BIV. A single C24 insertion in HIV-1 rewires loop–bulge communication to enable induced fit and higher Tat affinity, while HIV-2 TAR, with stronger self-integrity, favors conformational selection and weaker binding. Thermodynamic analyses reveal enthalpic stabilization in BIV versus entropic allostery in HIV-2, where loop breathing generates binding-competent ensembles. Extending beyond structure, solvation dynamics highlight a new allosteric layer: Tat binding quenches loop-bulge coupling in HIV-2 but enhances solvent-structure anticorrelated dynamics. Thus, solvation emerges as an allosteric avenue alongside structural communication, together defining how viral TAR RNAs diversify protein recognition and functional outcomes.

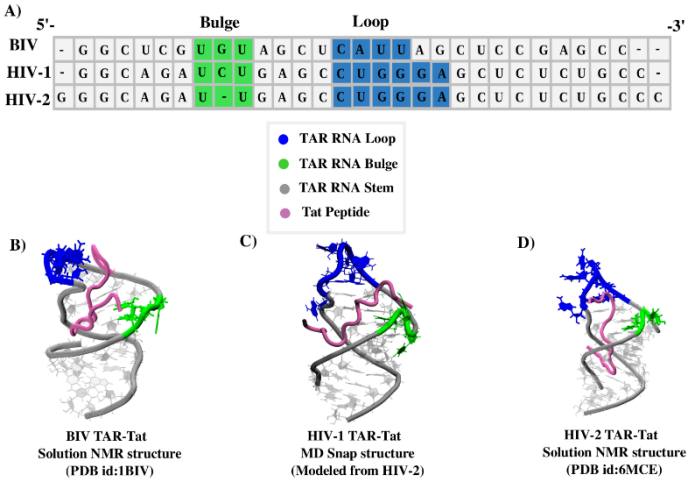


Figure 1 Comparing Different Variants of TAR RNA in the Tat-Binding Aspects. **(a) depicts the primary sequences in TAR RNA variants BIV, HIV-1 and HIV-2 respectively. (b), (c) and (d) show respective TAR-Tat complex structures.**

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STRUCTURAL INSIGHTS FROM PHOSPHORUS INCORPORATION INTO PORPHYRINS AND PYRIPORPHYRINS

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The non-innocence nature of porphyrins responsible for their redox behaviour in life processes results in tunable electronic properties, structural diversity and versatility in metal coordination[1]. Extensively studied for their bio-mimetic applications, recently single atom catalysts (SACs) mimicking the enzymatic reactions are reported with porphyrin or porphyrin-like moieties as the active unit[2]. Site specificity and tunability of catalytic functions can be achieved in these systems through electronic modulations[3][4]. In our work, we have explored the possibilities of substituting the nitrogen atom with phosphorus as well as expanding the framework by using pyrdine scaffolds instead of pyrrole which are further analyzed for phosphorous incorporation. Figure 1 shows some of the optimized geometries of tetra- and di- phospha substituted porphyrins and pyriporphyrins at B3LYP/6-31G* level of theory. The nature of out-of-plane (OOP) distortions has been characterized and the electronic reasons unearthed which can provide insights into the effective tuning of these molecules for desirable applications.

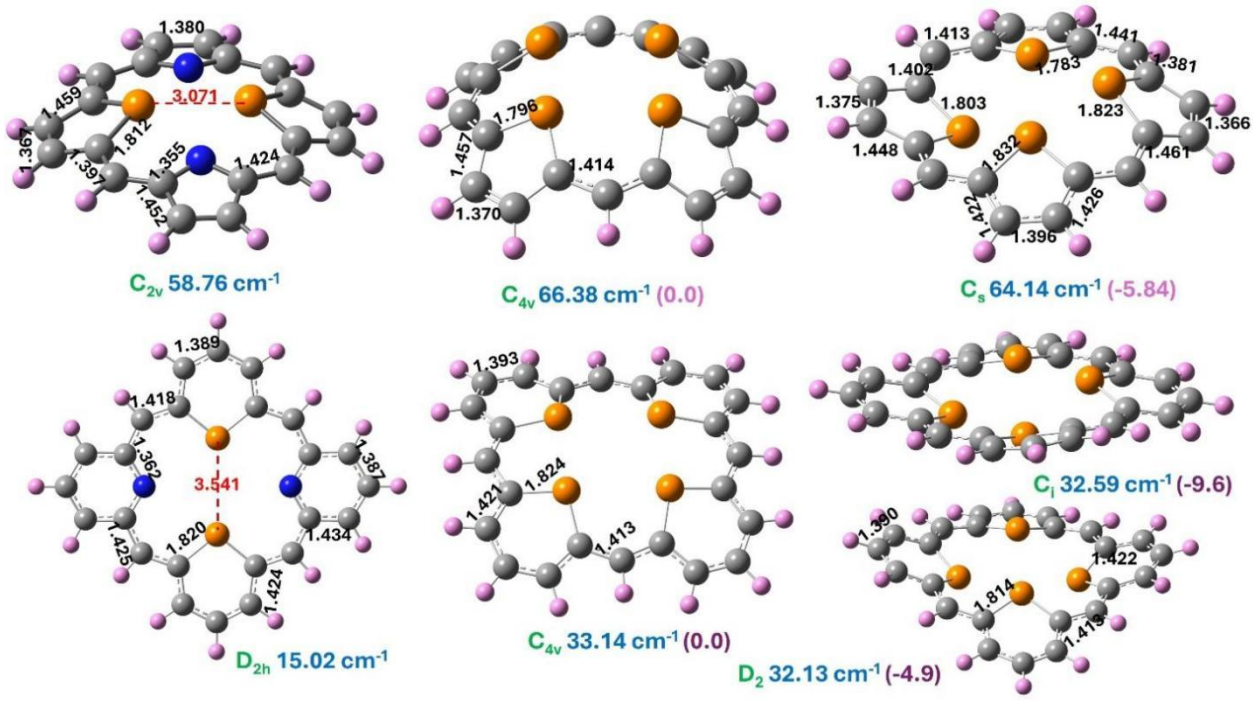


Figure 1. Phosphorus-substituted porphyrins and pyriporphyrins exhibiting various OOP distortions such as doming, waving, propellering and saddling. Optimized bond lengths, lowest frequencies and relative energies are given.

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A Computational Investigation of the Reaction between n-Propanol and Amidogen Radical (NH_2) in the Interstellar Medium

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The Interstellar Medium (ISM) is the space among the stars in our galaxy, where a wide range of attractive chemical reactions happen. It addresses the most fundamental questions about molecules that are responsible for the origin of life. To answer these questions, we carry out astrochemical modeling to understand the chemical routes for the evolution of planets and the formation of prebiotic molecules in the universe[1]. In the present work, we have done a detailed analysis of the gas-phase reactions between n-propanol and NH_2 in the ISM[2,3]. The investigation was initiated with the determination of stable conformers of n-propanol using post-Hartree methods like CCSD(T) and M06-2X with the Pople basis set 6-311++G(d,p). We located five distinguishable conformers of n-propanol that are also present in the ISM. The various reaction pathways involving the reaction of NH_2 radicals and five conformers in the ISM were explored at low temperature and low pressure. The energy profiles diagram for the given reaction was constructed using the CCSD(T)//M06-2X/ 6-311++G(d,p) level of theory. The rate coefficients were computed using the master equation approach and Rice-Ramsperger-Kassel-Marcus (RRKM) theory with Eckart tunneling correction implemented in the MESMER software package[4]. The global rate coefficients were obtained between 40 and 240 K, considering the Boltzmann population contributions from all conformers of n-propanol. Our study indicates that the rate coefficients are inversely dependent on temperature. Thus, our study provides a critical insight into the field of molecular evolution and suggests suitable reaction pathways for organic molecules with six or more atoms in the ISM via detailed kinetic investigation.

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Examining The First Electron Transfer Process in Pdx-Cytochrome $P450_{cam}$ Muti Site Binding Complex

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Cytochrome P450s are ubiquotes enzymes, known for its catalytic actions in drug metabolism, detoxification, and biosynthesis of natural products. The activity of P450cam is tightly coupled to a dedicated electron transfer chain composed of putidaredoxin reductase (PdR) and putidaredoxin (Pdx). In this system, electrons flow from NADH to the flavin adenine dinucleotide (FAD) of PdR, then to the [2Fe–2S] cluster of Pdx, and finally to the heme iron of P450cam. This sequential electron transfer, which holds the key to the catalytic cycle which is conserved for heme contating cytochrome monoxygeneses across the species, involves transfer of two electrons from Pdx to Heme,where the Pdx apart from being the redox partern also acts as the effector which controls the P450 conformational dynamics[1]. The Biological Electron Transfer involves a delicate choreography of protein-protein, protein-substrate, protein-solvent interactions[2]. In several Cytochromes it has been seen that the substrate binding has a considerble effect on the rate of electron transfer[3]. Recently a noble three site substrate binding mode was proposed for binding of camphor to the P450 enzyme[4]. In this study we examine the efffect which this proposed multi site binding mode imprts on the first electron transfer process and compare it with the conventional one site model.

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Theoretical Chemistry Symposium
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Thermodynamics of Protein-Ligand Binding

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Abstract
The study examines the thermodynamic interaction parameters between the covalent tyrosine kinase inhibitor Afatinib[1] and the Epidermal Growth Factor Receptor (EGFR), a crucial target in non-small cell lung cancer (NSCLC)[2]. Since covalent drugs have been utilized to treat a variety of malignancies, advancements in structural biology along with suitable simulation approaches are crucial to overcoming the difficulties in covalent drug discovery. Normal Mode Analysis (NMA)[3], Interaction Entropy (IE)[4], and the C2[5] method were used to calculate binding entropy contributions ($-T\Delta S$). Binding free energy of -19.86 Kcal/mole of the Afatinib-EGFR complex shows a better agreement with experimentally reported value of -13.00 Kcal/mole.

Table 1 Entropy estimated from the NMA, IE and C2 methods along with their calculated binding affinities, experimental binding affinity and experimental dissociation constant for the protein-ligand complex.

Complex	$T\Delta S_{NMA}$ (kcal mol^{-1})	ΔG_{bind} (NMA) (kcal mol^{-1})	$T\Delta S_{IE}$ (kcal mol^{-1})	ΔG_{bind} (IE) (kcal mol^{-1})	$T\Delta S_{C2}$ (kcal mol^{-1})	ΔG_{bind} (C2) (kcal mol^{-1})	K_d (Exp)	ΔG_{bind} (Exp) (kcal mol^{-1})
Afatinib-EGFR	-26.10	-19.86	-13.00	-32.96	-10.49	-35.47	0.1-1.1	-13.00 ±0.72

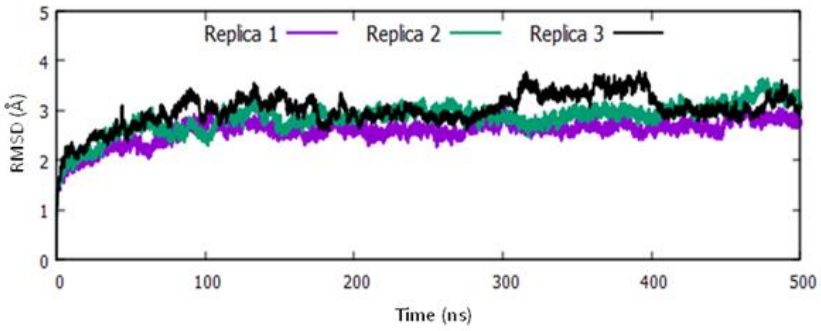


Figure 1 RMSD of the protein-ligand complex as a function of simulation time.

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Base Strength Guided In-silico Exploration of Mechanistic Pathway of Cholesterol to Cholest-5-en-3one oxidation

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Enzymes are biological catalysts which, unlike the traditional catalysts, perform its duty under milder conditions, with superior selectivity and high efficiency. In this aspect, biocatalysts are explored as an environmental friendly alternative to the existing ones. Conversion of cholesterol to cholest-4-en-3-one is one such platform where an enzyme, precisely Cholesterol Oxidase (ChOx), is used to facilitate a biochemical transformation. Cholesterol Oxidases (ChOxs) are bifunctional bacterial flavoenzymes that facilitate the oxidation of cholesterol to cholest-5-en-3-one and the subsequent isomerization of cholest-5-en-3-one into cholest-4-en-3-one[1]. It contains one mole of FAD(Flavin Adenine Dinucleotide) per mole of protein. The dehydrogenation of the substrate molecule involves the proton abstraction (3-OH) by a base and the hydride transfer (3-H) to the FAD molecule. Recent computational studies on ChOx from *Streptomyces SA-COO* species, considered Glu361 as the base, based on the extensive experimental studies[2]. The study identified that the proton abstraction and the hydride transfer occurs synchronously. In this study, we have tried to explore the dehydrogenation mechanism and energetics in the presence of strong and mild proton acceptors(base) using a miniature version of the substrate with the help of Density Functional Theory (DFT). Here, we have chosen the hydroxide(OH^-) and acetate(CH_3COO^-) ions to represent the strong and mild base respectively. The oxidation reaction is initiated by a spontaneous proton abstraction when the OH^- ion is involved while the hydride transfer occur simultaneously with the proton abstraction in the case of CH_3COO^- ion. Our work contributes an insight into how base strength can be a crucial factor in steering the mechanistic pathway of a reaction.

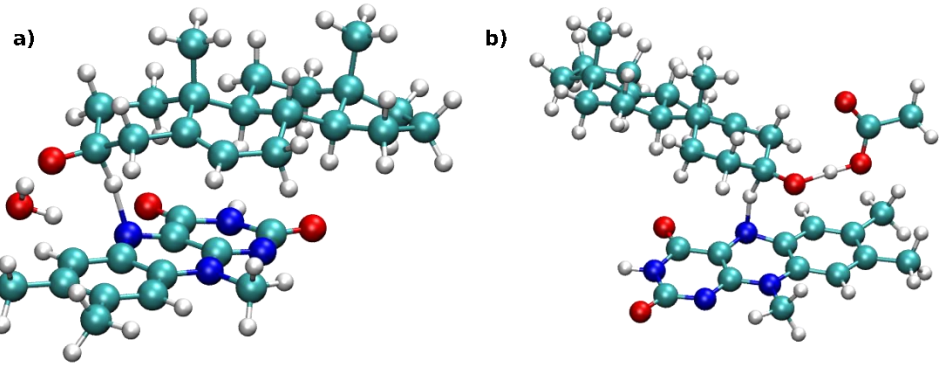


Figure 1: The dehydrogenation mechanism in systems with a) OH^- and b) CH_3COO^- as the proton acceptor. The system consists of the substrate molecule, which is a miniature version of cholesterol molecule, FAD and the proton acceptor.

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QM-Derived Atomistic Simulations Reveal How ssPalmO Derivatives Modulate Bilayer Properties for Lipid Nanoparticle Design

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The performance of lipid nanoparticles (LNPs) depends critically on how lipid chemistry and composition dictate bilayer organization, yet the underlying molecular determinants remain poorly defined. In this study, we use molecular dynamics simulations to characterize ssPalmO and its derivatives, and to investigate their properties to understand their potential as drug delivery materials for nucleic acids. Here, we combined density functional theory (DFT)-derived force fields with atomistic molecular dynamics (MD) simulations to investigate bilayers formed by ssPalmO, its phenyl (ssPalmO-phe) and benzyl (ssPalmO-ben) derivatives, and their cis/trans isomers. While most derivatives formed stable bilayers, cis-ssPalmO adopted a flexible non-lamellar structure, underscoring the destabilizing effect of stereochemistry. By contrast, trans isomers of ssPalmO-phe and ssPalmO-ben displayed enhanced bilayer thickness, packing density, and chain order due to conformational rigidity and stronger intramolecular interactions. Aromatic substitutions further suppressed lateral diffusion and reshaped electrostatic potential profiles, stabilizing the bilayers. Incorporation of helper lipids into cis-ssPalmO-phe bilayers synergistically improved packing, thickness, and electrostatic potential while reducing diffusion. Together, these findings reveal how functional group modifications, stereoisomerism, and lipid composition govern bilayer structure and dynamics, offering predictive molecular principles for optimizing LNP stability, encapsulation, and release. Our results complement recent reports on ssPalmO-based delivery systems [1,2] and align with advances in LNP engineering and self-assembly [3].

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AN EFFICIENT IMPLEMENTATION OF THE IMAGINARY-TIME PROPAGATION SCHEME FOR ACCESSING DIFFICULT ELECTRONIC STATES

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Imaginary-time time-dependent density functional theory (it-TDDFT) is a time propagation scheme in which the Kohn–Sham (KS) equations are evolved in imaginary time, efficiently projecting any trial wavefunction onto the electronic ground state. The it-TDDFT has been shown to converge systems that pose challenges for the standard self-consistent field (SCF) approach, reliably reaching the lowest-energy state that may remain inaccessible to conventional SCF procedures. Systems with small band gaps or degenerate single-particle energies often hinder efficient convergence with the traditional iterative methods, for which it-TDDFT provides an effective alternative.[1] In this work, we implement an efficient imaginary-time propagation scheme in NWChem to achieve a smooth convergence of difficult electronic states. The Chebyshev propagator is adopted for imaginary-time evolution owing to its convergence efficiency and inherent numerical stability.[2]

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Mechanistic Exploration of SO_2 Chemiluminescence Using Multi-Reference Methods

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Chemiluminescence (CL) involves the emission of light as a result of a chemical reaction.[1] Such process occurring inside a living organism is referred to as bioluminescence, with examples including firefly beetle, dinoflagellates and some fungi.[2] In most of the CL systems, light emission originates from the dissociation of a four-membered cyclic peroxide ring, where conical intersections near the ground-state transition state enable the molecule to populate multiple electronic states.[3] However, CL systems other than cyclic peroxides remain underexplored, and a general mechanistic framework of cold-light emission is still lacking. A recent theoretical study on air afterglow (NO + O) CL reaction revealed a distinct mechanism in which the ground-state pathway bifurcates via valley-ridge inflection, leading to the formation of NO_2 in the ground and excited electronic states.[4] Motivating from these insights, we are currently exploring the mechanistic details of SO + O reaction using multireference electronic structure methods such as CASSCF and CASPT2, combined with non-adiabatic dynamics. The study involves constructing potential energy surfaces (PESs), identifying minimum energy paths, and computing branching ratios among the accessible reaction channels. The SO + O system is expected to feature a rich and complex PESs involving both singlet and triplet electronic states. This scenario of multiple electronic states with different spin multiplicities is in contrast to the NO + O system and resembles with the cyclic-peroxide based CL processes. Our study, therefore, aims to understand whether the CL mechanism in SO + O aligns more closely with the former or the latter.

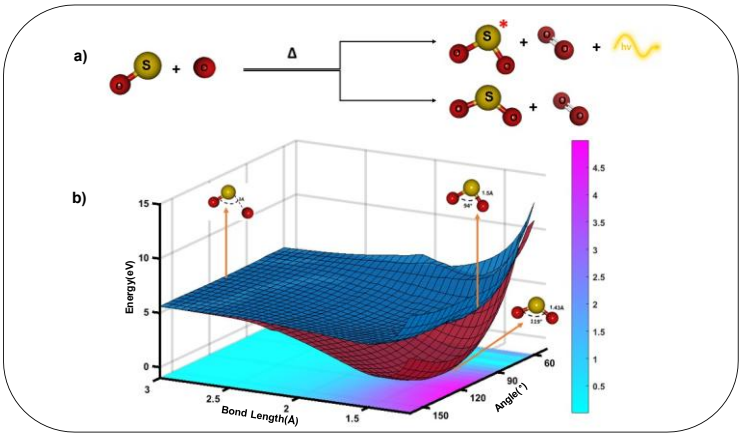


Figure 1 (a) CL reaction of SO + O forming SO_2 in both ground and excited states. (b) Rigid 2D scans describing SO_2 CL.

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Interfacial stability of Electrolytes at pure and oxidized Mg surfaces- Insights from Ab Initio Molecular Dynamics

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ABSTRACT

The development of high-performance magnesium batteries critically depends on salts that enable reversible Mg deposition. Among the leading candidates, $Mg(CB_{11}H_{12})_2$ offers excellent cycling efficiency but suffers from a high synthesis cost and impurity sensitivity. On the other hand, $Mg(TFSI)_2$, the only commercially available ether-soluble salt, undergoes electrode passivation and decomposition at Mg surfaces. Conflicting experimental and computational reports further obscure the role of surface heterogeneity on the stability of the salts. To resolve these discrepancies, we employ first-principles molecular dynamics to investigate the interfacial decomposition of $Mg(TFSI)_2$, $Mg(PF_6)_2$, and $Mg(CB_{11}H_{12})_2$ on three representative Mg anode models: pristine metallic Mg (m-Mg), stoichiometric MgO (s-MgO), and non-stoichiometric MgO (ns-MgO). We show that salt stability is strongly governed by oxide chemistry: while metallic Mg and stoichiometric MgO remain largely inert, non-stoichiometric MgO drives rapid anion decomposition and irreversible passivation. These findings establish surface heterogeneity as a key determinant of electrolyte performance and underscore the need for realistic surface models in guiding the design of next-generation Mg electrolytes.

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Novel Mechanistic Insights into Mn(II)-Catalysed Clauson-Kaas Reaction: A Density Functional Theory Study

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Pyrrole is an important aromatic heterocyclic scaffold found in many natural products and predominantly used in pharmaceuticals. Continuous efforts are being made to design and synthesize various pyrrole derivatives using different synthetic procedures.[1] Among them, the Clauson–Kaas reaction is a very old and well-known method for synthesizing a large number of N-substituted pyrroles. In recent years, due to global warming and environmental concern, research laboratories and pharmaceutical industries around the world are searching for more environmentally friendly reaction conditions for synthesizing compounds. Here we investigated novel mechanistic studies into Mn catalysed Clauson-Kaas reaction using density functional theory calculations. The model system involving 2,5-dimethoxytetrahydrofuran and aniline as reactants, with $Mn(NO_3)_2 \cdot 4H_2O$ as the catalyst, has attracted considerable attention due to its high coordination ability, low toxicity, low cost, and high activity.[2] The structures involved in the mechanism are optimized using 6-31G+(d) basis set and B3LYP functional in gas phase including D3 version of Grimme's dispersion correction. All calculations are performed in Gaussian 09 program. The work primarily focuses on the catalytic role of $Mn(NO_3)_2.4H_2O$ in Clauson Kaas reaction by investigating the site selectivity for the attack on 2,5-dimethoxytetrahydrofuran. Based on our studies, we have proposed a catalytic mechanism proceeding through Succinaldehyde and Imine intermediate for the investigated reaction.

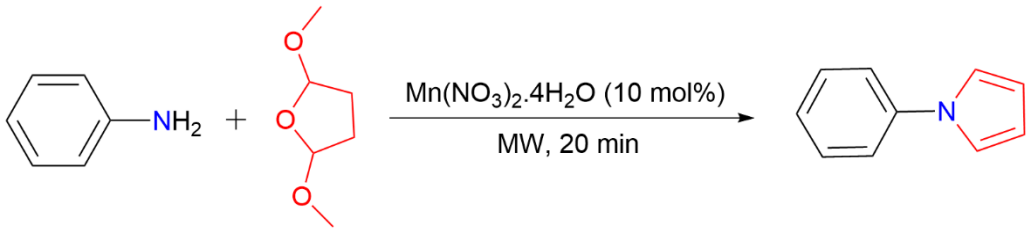


Figure 1 Model reaction of Mn catalysed Clauson Kaas reaction

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Role of *Naphthalene-to-Azulene* Reconstruction in Modulating Triplet Photosensitization in Chalcogenated Biazulenediimides and Reconstructed Perylenediimides

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Accessing and utilizing triplet excited states in purely organic molecules for applications in optoelectronics, display, photodynamic therapy, etc., are of important due to the increased energy efficiency and economic viability.[1] However, the large energy gap between excited singlet and triplet states (ΔE_{S-T}) and small spin-orbit coupling (SOC) hinder the intersystem crossing (ISC) and the reverse ISC (RISC) processes, limiting the triplet harvesting. Herein, the naphthalene based planar visible-light absorbing perylenediimide (PDI) dye and its functional derivatives are extensively studied for efficient triplet harvesting applications.[2-4] Interestingly, it's also of fundamental interest to gain insights on how the naphthalene replacement by its isoelectronic azulene unit modulates the PDI structure-function relationship, which remains unexplored. Installing azulene units results in two sets of systems, the analogous biazulenediimide (BAzDI) and the isoelectronic reconstructed PDI (*r*PDI). Further, the impact of chalcogenation on BAzDI and *r*PDI photophysics is also relevant for triplet harvest due to the expected heavy-atom effect driven SOC enhancement. Therefore, their chalcogenated congeners, termed as **X-BazDI**[5] and **X-*r*PDI**[6] (X=O, S, Se) are studied using density functional theory (DFT) and time dependent DFT (TDDFT) in dichloromethane and toluene dielectric, respectively, and results are compared and contrasted against the photophysical properties of **X-PDI** (X=O, S, Se) (See Scheme below).

Optimally tuned range-separated hybrid combining with polarizable continuum model in dichloromethane/toluene dielectric predicts reliable fundamental gap and low-lying excited state energies (adopting the 0-0 energy formalism) for the studied systems. The trend in the ISC rates (refer to the Table below) among **X-BAzDI** and **X-*r*PDI** as compared to **X-PDI** is well understood from the variation in SOC and ΔE_{S-T}. Diminished to completely turned-off fluorescence found for **X-BAzDI** and **X-*r*PDI**, respectively, is expected to improve the overall triple harvesting efficiency. Furthermore, the high energy first triplet excited state (T_1) predicted for both **X-BAzDI** and **X-*r*PDI** as opposed to lower energy T_1 of **X-PDI** signals to promising triplet photosensitization capabilities for both the systems. This study helps to understand the photophysics in azulene-based organic molecular systems including the structurally twisted ones, and provides molecular-design strategies for improving triplet harvesting propensity.

Scheme: Chemical structures of X-PDI, X-BAzDI, X-*r*PDI

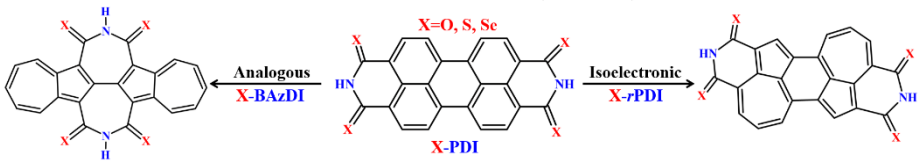


Table: ISC rates in s^{-1}

X	X-PDI[2-4]	X-BAzDI[5]	X-*r*PDI[6]
O	~0	~10^{7}	~10^{4}
S	~10^{11}	~10^{12}	~10^{5}
Se	~10^{13}	~10^{13}	~10^{12}

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BN Substitutional Influences on the Valence Isomers of Benzene: A Computational Study

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Boron–nitrogen (BN) substitution in aromatic frameworks provides a versatile approach to modulate stability and optical properties, yet its influence on benzene valence isomers has remained largely unexplored[1,2]. In this work, we investigated benzene, fulvene, benzvalene, Dewar benzene, and prismane using MP2 calculations with the aug-cc-pVDZ basis set under diverse BN substitution patterns (1BN, 2BN, and 3BN pairs). Our results show that BN incorporation enhances the stability of strained isomers, particularly Dewar benzene and benzvalene, with the greatest stabilization observed when B and N atoms are adjacent. In contrast, substitution patterns where B and N are separated by one carbon atom generally lead to destabilization, except in the case of benzvalene. Excited-state properties were further examined via TD-DFT/CAM-B3LYP calculations for the lowest three singlet and triplet states. Significant modifications in excitation energies and oscillator strengths were observed upon BN substitution, most notably in benzvalene and Dewar benzene, where enhanced optical activity was evident. Overall, our study demonstrates that BN substitution offers an effective strategy to tune both the relative stability and optical property of benzene valence isomers, highlighting their potential for optoelectronic and photonic applications.

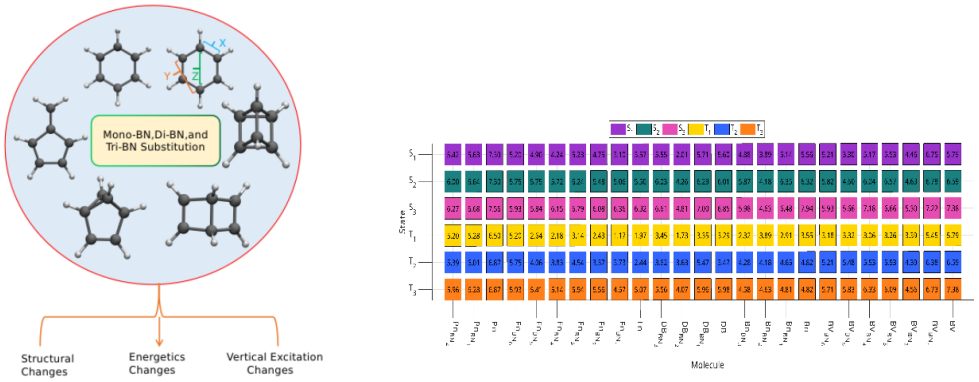


Figure 1 Comparison of Ground-state and Vertical Excitation energies (S1-S3 and T1-T3) for benzene and its valence isomers (benzene, fulvene, benzvalene, Dewar-benzene, and prismane) before and after BN substitution.

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Pore Electrostatic Potential Determines the Electrochemical Performance of Triazine-based Covalent Organic Framework Electrode in Lithium-ion Battery

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Covalent organic frameworks (COFs), an emerging class of layered, porous framework materials, have garnered significant recognition as an electrode material in metal ion batteries. The presence of redox-active functional groups, combined with structural tunability, opens opportunities for enhancing electrochemical performance in terms of storage capacity and voltage [1,2]. Using first principle simulations, we study a set of experimentally relevant triazine-based COFs, considering 1,4-Benzene, 1,4-Naphthalene, 2,6-Naphthalene, and 4,4′-Biphenyl as linkers, which differ by aromaticity and connectivity, to quantify the effect of pore electrostatic potential on the electrochemical performances of Li ion battery. We find that, due to the presence of different heteroatom-based binding motifs, the Li binding behaviour and the stepwise intercalation mechanism are significantly different compared to that of a conventional graphite electrode. We find that the voltage increases in the order 1,4-Naphthalene > 1,4-Benzene > 2,6-Naphthalene > 4,4′-Biphenyl, with a range of ~0.4 V. Furthermore, we have investigated COF systems with pore walls functionalized by -F, -CN, and -OH groups, revealing a strong dependency of pore ESP on the electron donating/withdrawing substituent group with an order of no substitution < F-substitution < CN-substitution > OH-substitution, resulting in further modulation of voltage. We find that such voltage modulation is controlled by the pore ESP of the COF, which concomitantly downshifts the CBM, eventually facilitating the electron transfer and the Li binding strength. Interestingly, Li migration in COFs is independent of the electronic or electrostatic factors; instead, it depends primarily on the rigidity i.e., on the nature of connectivity of the aromatic rings of linkers, where 4,4′-Biphenyl linker shows lowest barrier due to the possibility of free rotation around the central C-C bond, compared to that of rigid fused rings in naphthalene linkers. Overall, our study provides an in-depth understanding of the impact of ESP in triazine-based COFs in determining the electronic properties and thus influencing their electrochemical energy storage performance, opening up a route map in linker engineering aspects of the COFs.

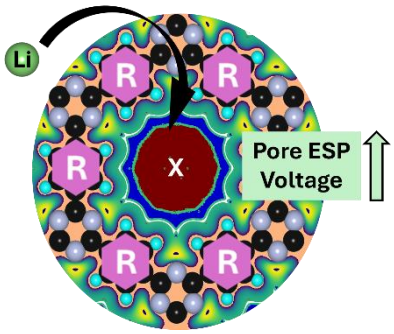


Figure 1 Schematic representation of Li intercalation in CTF-COF, depicting the pore electrostatic potential.

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Machine Learning Assisted Protein Design: A Random Forest Approach

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Computational protein design aims to predict amino acid sequences from scratch, without depending on natural templates, that will subsequently fold into a target three-dimensional (3D) structure and exhibit a specific function also termed as the inverse folding problem. Although traditional energy-based methods have significantly contributed to protein design, their computational expense and complexity often limit their application to small datasets or specific cases. In contrast, recent advances in machine learning have surely leveraged this field of computational protein design by capturing intricate relationship between protein sequences and their structures. In this study we developed a Random Forest model to evaluate its sequence design capabilities across input protein datasets with varying degrees of sequence similarities. Our motive is to examine how model performance gets affected and evaluating the stability under diverse sequence scenarios. Additionally, we examined the effect of balancing class distributions during training on predictive performance of the model. Our results suggest that predictive performance is significantly affected by input sequence similarity cut off, with higher similarity cut off often correlating with improved accuracy. Moreover, balancing class distributions enhanced classification performance by mitigating bias introduced by imbalanced class distribution. These observations emphasizes the dual importance of both sequence diversity and data balancing strategies in building generalizable and interpretable machine learning models for protein design. Across all datasets proline and glycine exhibits highest prediction accuracy and persistent confusion lies in differentiating hydrophobic residues (leucine, isoleucine and valine) probably because of the evolutionary exchangeability of the three amino acids. The insights gained from this study may aid in the advancement of computational approaches to protein design.

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Phase Transformation in Silicon: Anomalies Revealed by Computational Free Energy Analysis

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Silicon holds critical importance as both a technological and structural material. In this study, the melting mechanism of silicon is systematically investigated using molecular dynamics (MD) simulations with the Stillinger–Weber[1] (SW) potential, emphasizing free energy analysis. A first-order solid–liquid phase transition is proposed to elucidate silicon's anomalous behavior. Unlike conventional substances, silicon exhibits a density anomaly: a sharp density drop during quenching and an abrupt increase upon heating[2]. The liquid–liquid transition (TLL) is identified at ~1375 K, characterized by a change in the first-shell coordination number from ~8 to ~5 with decreasing temperature (Fig. 1). During quenching, the tetrahedral order parameter rises markedly from 0.57 to 0.92 near 1050 K, signifying the nucleation of the diamond crystalline structure. Free energy differences between phases are quantified using a three-stage reversible thermodynamic cycle, with multiple histogram reweighting[3] (MHR) applied to extract the equation of state. The free energy difference near the melting point is −0.3520 ± 0.0135 kJ/mol. The solid–liquid coexistence temperature is estimated as 1673 ± 5 K. Furthermore, the melting line obtained from Gibbs–Duhem integration reveals a negative slope, with a coexistence line gradient of approximately −61.7 K/GPa, indicating a pressure-induced reduction in melting temperature.

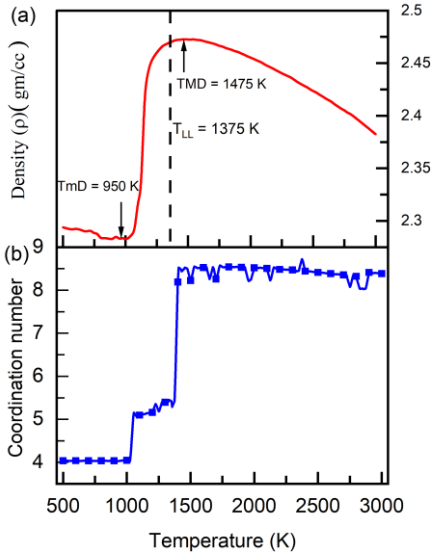


Figure 1: (a): The density of Silicon as the temperature is lowered during the cooling process. Arrows demonstrate the density maximum at 1475 ± 10 K(TMD) and the density minimum at 950 ± 25 K(TmD). The perpendicular dash line marks the liquid-liquid transition temperature, T_{LL} = 1375 ± 25 K. (b): First shell coordination number (CN) as a function of temperature during the quenching process.

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Leveraging High-Spin DFT Features for Prediction of Spin State Gaps in 3d Transition Metal Complexes

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Determining spin state energy gaps (SSE) of 3d transition metal complexes (TMCs) is a major challenge in theoretical chemistry, as high-level quantum methods, though reliable, are computationally impractical for large-scale studies[1]. This work explores a machine learning (ML)-based approach to predict DFT adiabatic SSE gaps using descriptors derived from a single high-spin DFT calculation. This approach is adopted to eliminate the differential treatment of electronic correlation between high-spin and low-spin structures.

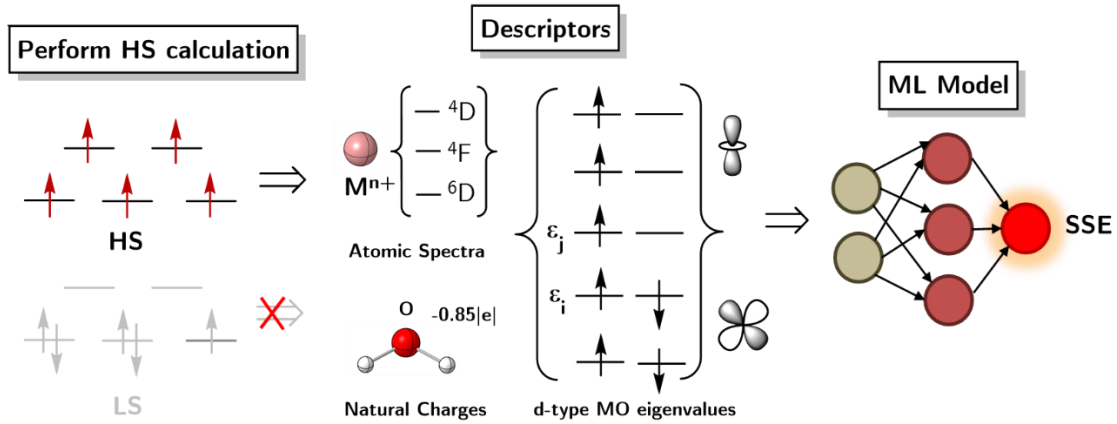


Figure 1 Representative diagram of the ML study alongwith workflow and descriptors.

Our descriptors aim to incorporate the knowledge of crystal field theory into the ML model. They include atomic energy levels of bare metal ions, natural charges of ligating atoms, d-orbital molecular orbital eigenvalues derived from an high spin calculation, HOMO–LUMO gaps of free ligands, and simple identity-based features. We train ML models on 1434 SSE values spanning 934 complexes[2] and demonstrate their transferability to more challenging complexes having bidentate π-bonding ligands despite being trained on simpler Werner-type monodentate complexes. We achieved a minimum MAE of 4.0 kcal mol^{-1} on the monodentate test set, and maintained a comparable MAE of 6.6 kcal mol^{-1} in the transferability assessment[3]. This approach bypasses the need for multi-reference low-spin optimizations while retaining predictive accuracy, offering a cost-effective strategy for SSE estimation in transition metal chemistry.

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A Theoretical Study on the Dynamics of Highly Energetic Nitrogen Isotopic Exchange Reactions

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The dynamics of the $^{14}N + {}^{15}N^{15}N$ exchange reaction is investigated by employing the time dependent wave packet propagation method[2,3,4,5,6] on the ground electronic $N_3(^4A'')$ potential energy surface[1]. We focus on ortho- $^{15}N^{15}N$ (j = 1) and para- $^{15}N^{15}N$ (j = 0) configurations, analyzing the formation of meta-stable quasi-bound complexes and comparing reaction thresholds and probabilities. The influence of total angular momentum and initial vibrational levels on reaction dynamics is assessed for both *ortho* and *para* states. Furthermore, the integral cross-section is also observed and compared for both states.

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THEORETICAL STUDIES OF MAGNETIC EXCHANGE COUPLING IN SELECTED POLYNUCLEAR TRANSITION METAL-METAL COMPLEXES

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The study of magnetic properties in coordination compounds is one of the most important areas of research as it provides fundamental insights on electronic structure, bonding and applications as spintronic devices. Especially metal–metal complexes represent an important class of compounds where two or more transition metal centers are linked through direct bonding interactions[1,2]. Broken-Symmetry DFT is carried out in polynuclear metal-metal complexes to study the anti-ferromagnetic coupling by calculating exchange coupling constant (*J*) which is fundamental to understand spin spectra of magnetic system[3]. When both metal ions have unpaired electrons then intramolecular spin exchange interactions and ferromagnetic or antiferromagnetic coupling arises. Exchange interaction can be satisfactorily described for metals of first transition series by Heisenberg-Dirac-van Vleck model with the spin-Hamiltonion operator $\mathbf{H=-2JS_1.S_2}$, here S_1 and S_2 are the total spins on metal 1 and metal 2[4]. The positive value of J indicates ferromagnetic coupling whereas negative value is for antiferromagnetic coupling. So, we have calculated Exchange coupling constant (*J*) for various complexes with polynuclear metal-metal linkage and compared the *J* values calculated by different DFT methods (such as, B3LYP, wBP97xd, M06, PBE, TPSS, etc) and *ab-initio* methods with experimental values.

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First-Principles Insights into the Structural and Electronic Behavior of B_2C for Post-Lithium-Ion Energy Storage

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In recent years, two-dimensional (2D) materials have garnered considerable research interest due to their unique properties and potential application in energy storage. One of these materials, B_2C, demonstrates promising characteristics making it a strong candidate for use as an anode in metal-ion batteries, particularly calcium-ion and potassium-ion batteries (CIBs and KIBs)[1,2]. The rising attention towards CIBs and KIBs as alternatives to lithium-ion batteries (LIBs) is primarily motivated by the greater availability and lower cost of calcium and potassium as compared to lithium[3]. Nevertheless, finding suitable electrode materials for these batteriy systems remains a major challenge.

In this study, first-principles calculations were employed to examine the electronic and structural variations within B_2C during metal ion intercalation. The Climbing Image Nudge Elastic Band (CI-NEB) method was used to determine the diffusion barriers for the migration of Ca/K ions onto B_2C[4]. The calculated diffusion barriers were notably low, at 0.14/0.07 eV for Ca/K migration (Figure 1). The results also indicate that, B_2C exhibits an excellent Ca/K storage capacity, along with good electronic conductivity and robust structural stability during calcination and potassination processes. Molecular dynamics simulations have also been performed to study the thermal stability of pristine as well as metal loaded B_2C. These findings suggest that B_2C holds substantial potential as a high-performance anode for next-generation CIBs/KIBs, offering potential for more efficient and sustainable energy storage technologies.

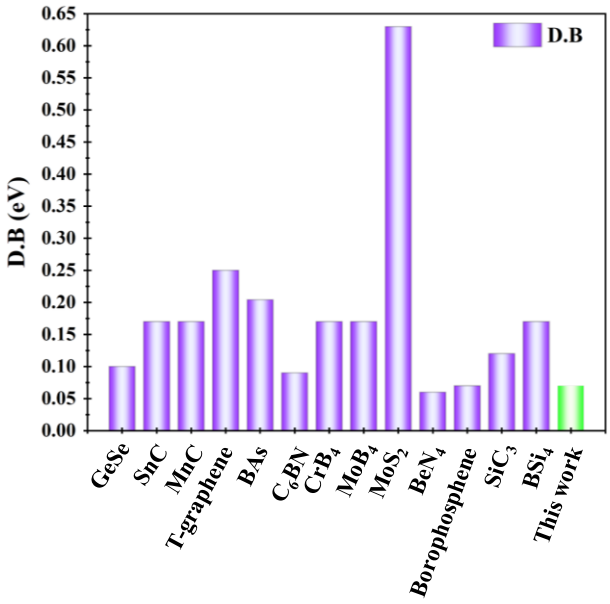


Figure 1 DFT based calculated diffusion barriers for some of the reported 2D anodes for KIBs.

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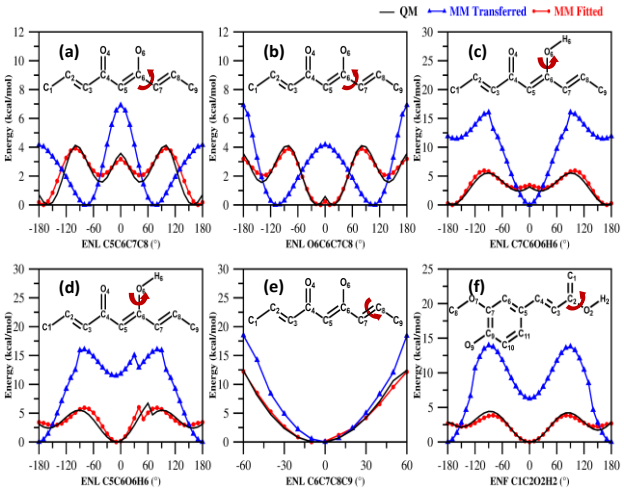
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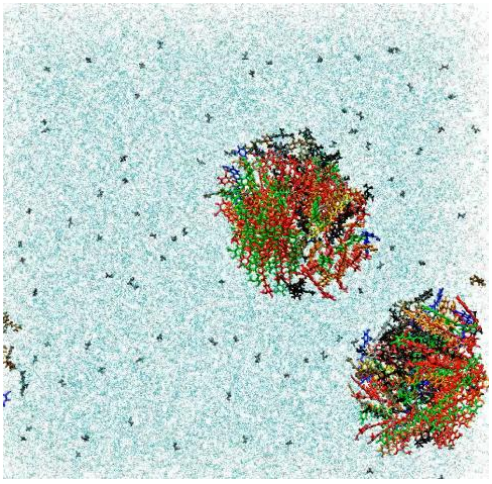
Enhancing Ayurvedic Phytochemical Research with Force-Field Parameterization for Diverse Applications

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Ayurvedic phytochemicals have therapeutic potential, but their mechanisms remain unclear due to limited computational models. This study develops accurate force-field parameters for major phytochemicals present in *Haridra* (*Curcuma longa*) using protocol devloped in CHARMM General Force Field (CGenFF)[1] parameterization involving QM/MM vibrational comparisons, energy scans, and non-bonded interaction optimization validated by experimental data. The approach will extend to ayurevdic herbs like *Amla*, *Guduchi*, and *Vasa*, with molecular dynamics simulations used to explore their synergistic effects.

`MD simulations have been conducted for *Haridra*, including simulations of its key phytochemicals (curcuminoids and turmerones), which mimic the molecular profile of *Haridra*. These simulations study the aggregation behavior and interactions of these phytochemicals, providing insights into their therapeutic mechanisms.





(a) (b)

Figure 1 (a) Potential Energy Surface (PES) scans used for fitting dihedral parameters during force-field development. (b) Aggregation behavior of curcuminoids studied through molecular dynamics simulations

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Underlying Mechanisms of Hydrophobic Tripeptide Self-Assembly Revealed by Event-Tracking and Free Energy Calculations

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Self-assembly of ultrashort peptides is an important topic in contemporary soft-matter research[1]. We investigated the mechanistic pathways leading to the final self-assembled states of three tripeptides—phenylalanine tripeptide (FFF), leucine tripeptide (LLL), and isoleucine tripeptide (III)—using our in-house developed **Event-Tracking algorithm**[2]. This algorithm enabled us to capture fusion and fission events among peptide clusters during the dynamical assembly process. Our analysis revealed that the assembly mechanism of FFF is the most hierarchical, that of III the least hierarchical, with LLL displaying an intermediate behaviour. To rationalize these differences, we examined bimolecular association via umbrella sampling simulations[4]. The formation of a **middle-to-middle hydrogen bond** emerged as a key stabilizing factor in dimerization. Due to its geometry, the III molecule favoured this bonding mode, while FFF was less inclined to form such interactions. LLL, consistent with its intermediate behaviour, showed moderate preference. These distinctions were further supported by brute-force simulation data analyzed using our **TAMCIS (Temporal Analysis of Multidimensional Chemical Interaction Space)** method[3]. TAMCIS allowed us to identify the specific chemical interactions driving the assembly process, corroborating the differential mechanistic pathways observed for the three peptides.

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4 A. Chakraborty and A. Das* (Under Preparation)

Theoretical Chemistry Symposium
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Computational Framework to Describe Photo Induced Charge Transfer Excitations in Non-Chromophoric Protein Systems

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Over the past few years, we have observed very unusual spectral signatures in near-UV and visible range from biomolecules such as amyloid aggregates[1] and different proteins[2,3]. The origin of such spectral signatures is very unclear as they don't possess well defined chromophores/fluorophores. Understanding the fundamental processes behind such anomalous observations is crucial as it could lead to the development of label-free probes to study biological processes in-vitro and in-vivo. Recently our group has developed a computational framework based on classical MD simulations, TDDFT calculations, and population analysis schemes to identify photo-induced charge transfer (PICT) transitions in clusters of oppositely charged residues as a key contributor to these anomalous absorption signatures using $\alpha 3C$ as a model protein[4]. However, the earlier framework struggled to capture the high-energy region and simulate full spectral profiles. Here, we present an improved method that accurately describes transitions across all energy ranges. In addition, we introduce electronic decoupling distance as a criterion to define the size of a charged residue cluster as an effective chromophore and apply this model to study spectral changes induced by protein acetylation, a common post-translational modification.

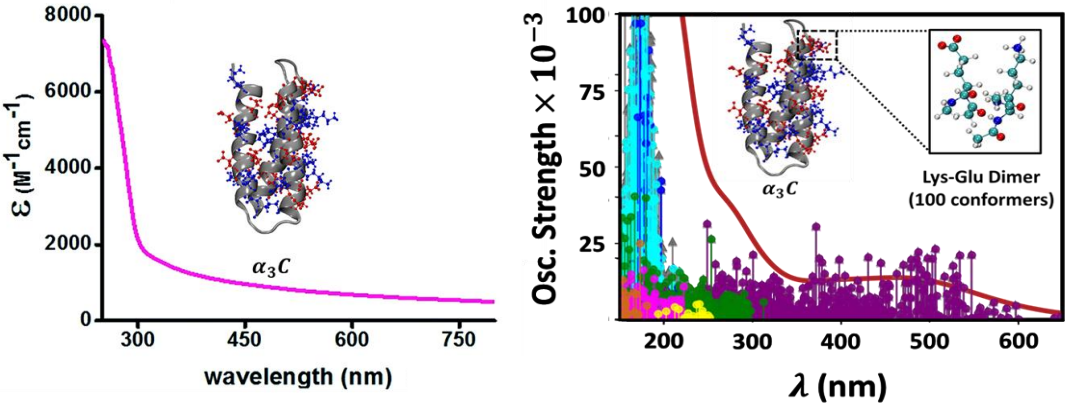


Figure 1 : Characterization of UV-visible spectra of $\alpha_3 C$ protein using Lys-Glu dimer as a model system. Different coloured transitions are represent different donor-acceptor groups in the CT transitions.

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Decoupling Nonlinearity and Transparency: A Through-Space Charge Transfer Approach for Advanced Optical Materials

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A major challenge in designing nonlinear optical (NLO) materials is that maximizing the NLO response often compromises optical transparency. In standard donor-π-bridge-acceptor (D-π-A) molecules, the through-bond charge transfer (TBCT) used to enhance NLO properties[1,2] also causes a strong red-shift in absorption, significantly reducing the transparency of material. This study investigates a molecular design aimed at overcoming this trade-off. We focus on a cofacial π-bridge architecture that allows charge transfer to occur through two different pathways at the same time: the conventional TBCT and a cofacial through-space charge transfer (TSCT). While this TSCT approach has been studied,[3] effectively using it to balance efficiency and transparency has been difficult. Our computational analysis shows how these two pathways interact. We find that the TBCT path is still the main driver of the NLO response. However, the TSCT channel plays a key dual role. It actively contributes to the overall NLO enhancement while also suppressing the unwanted red-shifting of the main absorption peak. This dual functionality allows for a much improved balance, optimizing NLO performance while keeping the material transparent. This work provides a practical path for developing new NLO materials needed for applications like optical limiting.

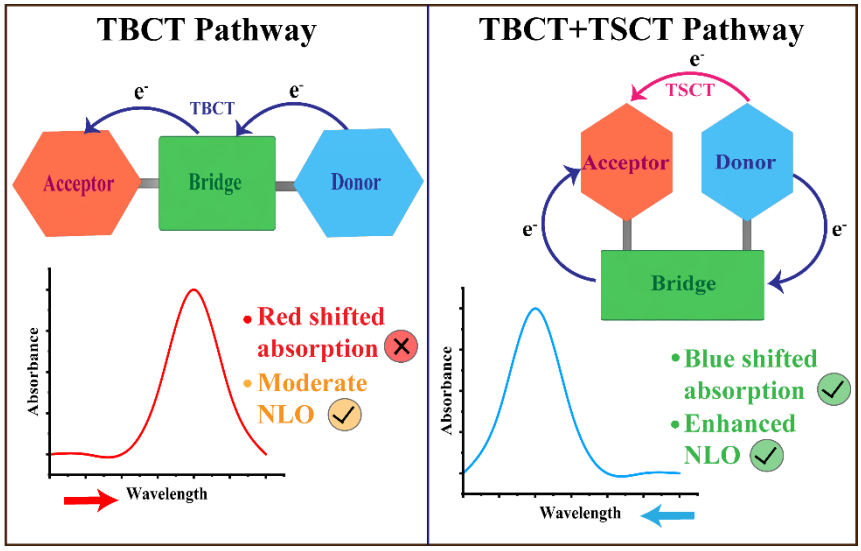


Figure 1 Comparison of traditional TBCT and combined TBCT+TSCT pathways. The TBCT-only pathway (left) leads to excessive red shifted absorption and limited control over optical transparency. Incorporating an additional TSCT pathway (right) effectively balances the optical transparency while retaining high NLO activity.

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A Novel semiconducting 3D Graphene with Acetylide Crosslinks

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Following the advent of 2D Graphene, 3D graphene, i.e., graphene selectively connected across layers, has been receiving unprecedented attention over the past decade. In addition to the robust properties and excellent stability of graphene, the interlinking of layers avoids overstacking/poor accessibility, and also addresses the problems associated with a zero band gap by prudent choice of linking sites. An ideal 3D graphene should retain the desirable properties of graphene in usable macroscopic materials. To address this challenge, we have designed a 3D graphene by vertically stitching with acetylide linkages alternating on either side of the graphene to retain the aromaticity and periodicity in the third dimension. The high D_{6H} symmetry was retained to utilize the strength of aromatic sextet rings, which gives a ratio of 1:3:1 for sp, sp^2, and sp^3 carbons, respectively, for this. Our DFT calculations (GGA/PBE, 440eV plane wave cutoff) on this novel carbon allotrope (z = 20) with a hexagonal unit cell (P6/mmc, No. 194) reveal an indirect band gap and are 12.5 kcal/mol less stable than graphene per carbon. Both valence and conduction bands, are dominated by sp^2 carbons as revealed by the projected DOS, despite the presence of reactive acetelide groups, presumably due to the non-planarity of the aromatic ring.

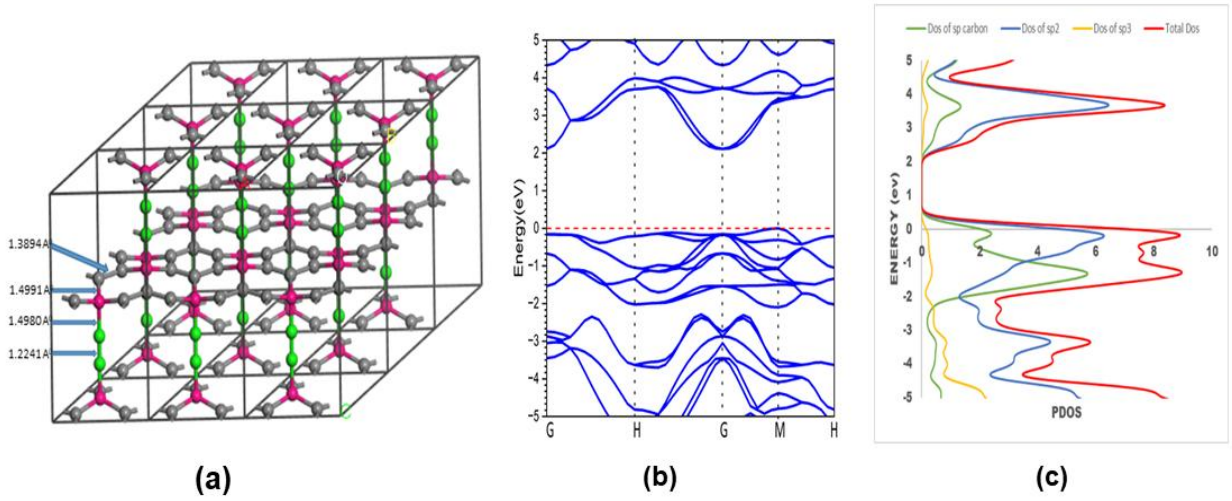


Figure 1.(a) the unit cell (P63/MMC) with SP carbon as green, SP^2 carbon as gray and SP^3 carbon as pink (b) its electronic band structure and (c) projected density of states (PDOS) of SP carbon(green), SP^2 carbon(blue), SP^3 carbon(yellow).

The material may have applications in various technologically important domains, including optoelectronics, solar cells, photovoltaics, and visible light emitters. It can also be used in designing the electrodes and supporting electrolytic reactions.

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Decoding DNA flexibility in Cren7-DNA Complex via Molecular Dynamics Simulations

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Cren7, a conserved chromatin protein in Crenarchaeota, organizes and stabilizes genomic DNA. A few investigations have already been performed regarding the stability of Cren7-DNA on the binding of Cren7 to DNA using MD simulations. The conformational dynamics of DNA in the Cren7-DNA complex are still unexplored. Molecular dynamics simulations were carried out to investigate the conformational dynamics of DNA in the Cren7–DNA complex. Both the wild-type (WT) protein and four aromatic mutants (W26A, F41A, F50A, and Y58A) were examined to assess their effects on DNA structural stability. Cren7 binding induced bending of DNA in both WT and mutant complexes, although the extent of bending varied. The mutants exhibited enhanced bending compared to WT. In parallel, hydrogen bonding between base pairs was perturbed during the simulations, consistent with conformational rearrangements of the DNA helix. Alterations in base stacking interactions further highlighted changes in DNA stability. Analysis of intra-base pair and base-pair step parameters revealed notable deviations in the mutants relative to WT. These changes were accompanied by modifications in backbone dihedral angles as well as in groove width and depth, reflecting global perturbations in DNA architecture. This study demonstrates how mutation in protein can induce change in conformations and flexibility of DNA via non-covalent interactions in a protein-DNA complex.

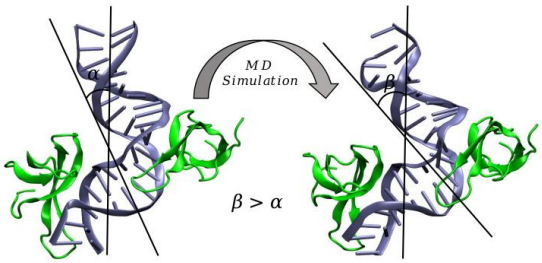


Figure 1 A change in DNA bending in the mutant F41A is reperesented via MD snapshots.

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Ab Initio Modelling of Spin Relaxation in Metal-Organic Framework-based Qubits

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Molecular qubits based on extended coordination frameworks represent one of the latest frontiers of spin-based quantum sensors or qubits, where long spin coherence times are combined with chemical versatility. The electronic states and vibrational modes of these frameworks carry sufficient information, which eventually exhibit long coherence time to behave as qubits. Here we employed ab initio spin relaxation theory to fully investigate the role of one- and two-phonon processes to understand the spin-phonon relaxation of vanadyl tetraphenylporphyrinate MOF, namely in [VO(TCPP-Zn_2-bpy)].[1] Here, we used the ab initio spin relaxation theory[2] to simulate the spin-lattice relaxation time (T_1) using NEVPT2(1,5) and NEVPT2(9,9) methods. Expanding the active space from d-d excitations to metal-ligand bonding orbitals[3] clearly shows an improvement in the spin-dynamics, emphasizing the use of the full electronic Hamiltonian instead of the effective Hamiltonian formalism, where the latter is often used as a standard method in lanthanide complexes.

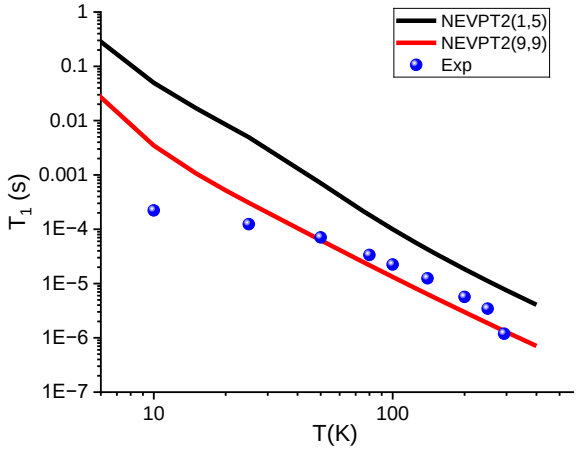


Figure 1 Comparison of the experimental and ab initio spin-lattice relaxation time (T_1) for the VOTCPP MOF using different active spaces.

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Computational Study of effect of progressive p-Sulfonation at upper rim of Calix[4]arene on adsorption with small gaseous molecule.

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Complexation property of calixarene with various charged ions, drugs and neutral gaseous molecules is an old-age concept. Here, in present work we are performing theoretical calculations to understand the complexation of CO_2 molecule with biologically important supramolecule i.e. p-sulfonatocalix[4]arene (SC4A). We have performed a comparative study to check the stability of guest small molecule in unsubstituted calix[4]arene (C4A) and simultaneously with various sulfonatocalix[4]arene (SC4A) receptors. Also discussed how solvent environment specifically polar solvent affect the inclusion of guest molecule. Theoritical calculations like equilibrium geometry optimization, vibrational spectroscopy, global reactivity descriptors, themodynamic quantities and adsorption energy calculations led us to the result that HOMO-LUMO gap increases upon complexation of CO_2 with chosen receptor, adsorption energy of guest CO_2 molecule i.e., stability increases with progressive sulfonation[1].

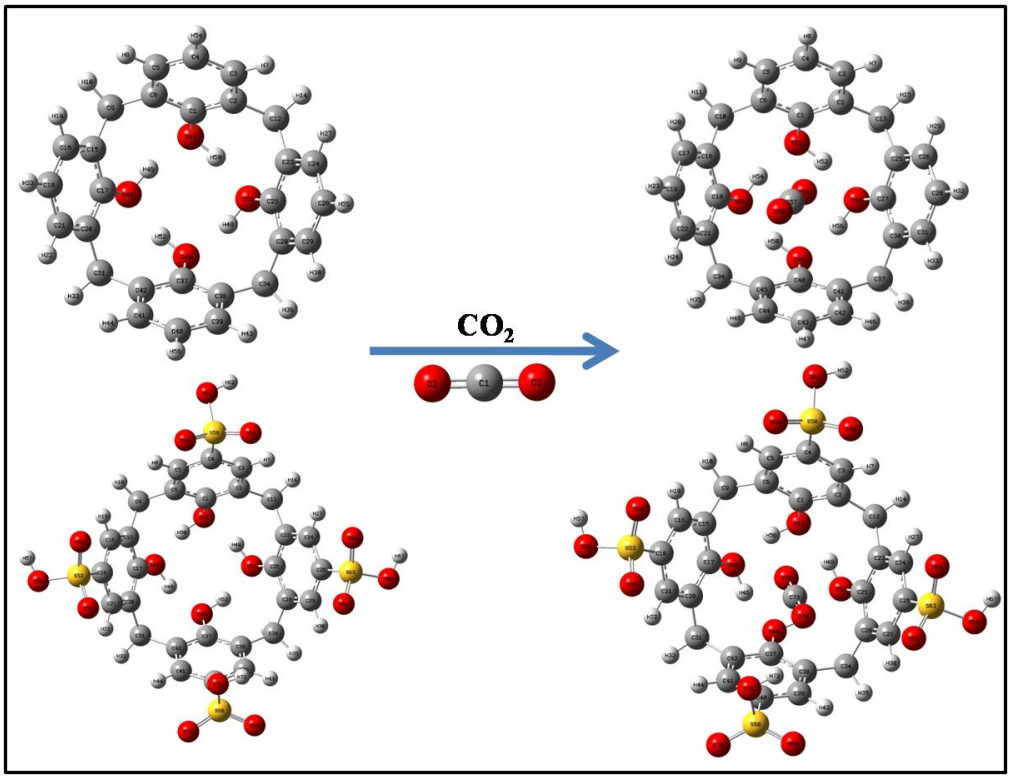


Figure 1: Inclusion of gaseous CO_2 molecule with chosen receptor molecules.

References:

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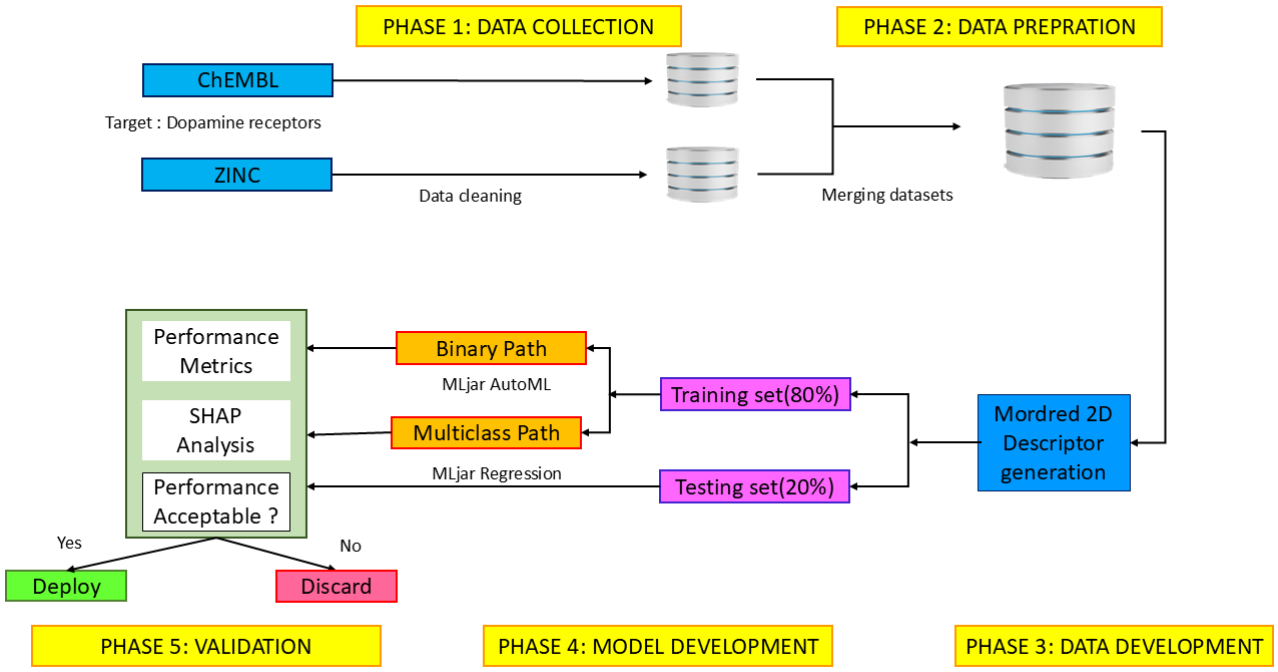
Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Ligand-Centered Machine Learning for Dopaminergic Activity and Receptor Subtype Selectivity

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Dopaminergic signalling depends on a heterogeneous family of receptors DRD1–DRD5, and transport/metabolic proteins that regulate extracellular dopamine. we describe a ligand-based machine-learning approach to differentiate compounds that exhibit measurable dopaminergic activity and privilege receptor subtype selectivity, based exclusively on two-dimensional molecular descriptors. In this work, records were aggregated from multiple bioactivity repositories, harmonized across identifiers, de-duplicated, and standardized at the target level to ensure data quality and consistency. The resulting dataset captured both agonists and antagonists across receptor families, enabling the development of a balanced model. The models generalized well to held-out compounds and highlighted physicochemical and graph-topological properties as salient determinants of activity, with selectivity signatures distinguishing major receptor families. Furthermore, analysis of feature importance suggested that molecular polarity, aromaticity, and connectivity indices play critical roles in shaping subtype-specific binding profiles. Taken together, these results demonstrate that simple descriptor-driven machine learning approaches can effectively capture complex structure–activity relationships in dopaminergic systems, providing a scalable framework for prioritizing chemical matter in early-stage drug discovery in the future.

Figure: Overview of the workflow.



Optical Properties of Metal Nanostructures: From Monomer Polarizabilities to Dimer Responses via Analytical Approximations

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Localized surface plasmon resonances (LSPRs) in noble metal nanoparticles are characterized by the collective oscillation of conduction electrons in response to an external electromagnetic field. LSPRs yield distinct spectral absorption and scattering peaks, along with intense electromagnetic near-field enhancements[1], facilitating diverse applications in nanophotonics. Analytical and semi-analytical modeling approaches have contributed immensely to our current understanding of plasmonic properties. Numerical methods such as the finite-difference time-domain (FDTD) method, finite-element method, and discrete dipole approximation are also commonly employed to investigate optical phenomena associated with LSPRs. In the quest for an accurate description of the optical features of metal nanostructures, a hierarchy of modeling approaches beyond the quasi-static approximation have been explored. Herein, we present an assessment of the accuracy of the approaches based on quasi-static approximation and modified long-wavelength approximation for the description of LSPR features of monomers and dimers of spheroidal and core-shell nanostructures by benchmarking against data from the FDTD simulations[2-5]. The dimers have been modeled within the framework of the coupled dipole approximation[6,7]. The accuracy of these analytical approaches relative to FDTD is limited at very small interparticle separations, but the analytical predictions progressively align with the FDTD results as separation increases. Our findings[8] suggest that the approximate approaches offer a lucid description of the optical response exhibited by the considered nanostructure dimers at larger interparticle separations and can be implemented at fairly low computational costs.

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Computational Insights into the Confined Hydrogen Evolution Reaction in Graphitic Systems

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The development of catalysts for the sustainable and energy-efficient valorization of small molecules has gained much attention in recent years. Among the various approaches, 'confined catalysis'–where the catalytic process occurs within a unique chemical environment created by confinement in the catalytic system–has emerged as a particularly effective strategy, as it can significantly enhance the activity, selectivity, and stability of catalysts for small molecule activation[1]. For instance, numerous efforts have been made to employ confined catalysts to improve reactions such as CO_2 and syngas conversion, water splitting-which is comprised of the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER)[2,3] etc. 'Catalysis under 2D-cover' is an emerging approach of catalysis in which chemical reactions take place in the confined space between a 2D material (such as h-BN, MoS_2 or graphene) and the surface of underlying support like metals or semiconducting oxides. Despite a plethora of research over the years, a deeper understanding of the role of spatial/electronic confinement, structural and electronic properties of the scaffolds employed, and specific reaction conditions are elusive. Various studies have been conducted to enhance catalysis for various reactions by employing structural engineering techniques, such as doping, in these 2D materials[4]. It was found that defects-enriched graphene-based electrocatalysts show great potential to replace the expensive and rare noble metal catalysts due to their excellent activity and low cost[5]. In this study, we employed density functional theory (DFT)-based computations to scrutinize the possibility of using various graphitic systems as confined catalysts for HER and scrutinized the role of spatial/electronic confinement in determining its catalytic activity. Our findings highlight that the charge density distributions play a crucial role in graphene-graphene interface chemistry and can be effectively tuned through suitable dopants, defects, or their combinations to achieve optimal HER activity.

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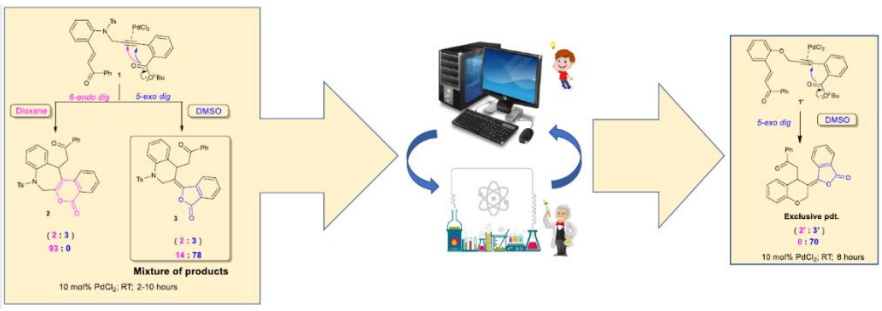
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Pd-Catalyzed Intramolecular Oxypalladation-Initiated Domino Reactions: Why does Solvent Polarity Control the Regioselectivity?

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Pd-catalyzed intramolecular oxypalladation-initiated cascade of internal alkyne **1** bearing *N*-tosyl tether can give rise to either functionalized benzazepine **2** via 6-*endo-dig* pathway or tetrahydroquinoline scaffold **3** via 5-*exo-dig* pathway. Surprisingly, the outcome of the reactions is found to be solvent-dependant. While 6-*endo-dig* was the exclusive pathway in 1,4-dioxane solvent, both the 5-*exo-dig* and 6-*endo-dig* pathways were found to be parallelly operative in DMSO.[1] In order to understand the role of the solvent in controlling the regioselectivity, Density Functional Theory (DFT) analysis was performed. DFT analysis have shown that formation of the *σ*-vinylpalladium intermediate can be reversible for the 5-*exo-dig* pathway while it is irreversible for the 6-*endo-dig* pathway in 1,4-dioxane. As a result, the 5-*exo-dig* pathway is found to be unproductive in dioxane. The formation of the *σ*-vinylpalladium intermediate is irreversible for both 5-*exo-dig* and 6-*endo-dig* pathways in DMSO solvent, and, as a result, both pathways are found to be productive in DMSO solvent. DFT predicted that the replacement of the *N*-tosyl tether by *O*-tether in the alkyne substrate may stabilize the *σ*-vinylpalladium complex for 6-*endo-dig* pathway in DMSO solvent, and consequently an exclusive formation of isobenzofuranone-fused chromane **3´** from *O*-tethered internal alkyne substrate **1´** is predicted via 5-*exo-dig* pathway. The experimental study confirms the theoretical hypothesis.



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Unlocking Inverted Singlet–Triplet Gap in Alternant Hydrocarbons with Heteroatoms

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With the growing interest in diverse material systems for organic light emitting diodes (OLEDs), multiresonant thermally activated delayed fluorescence (MR-TADF) compounds have attracted considerable attention due to their unique photophysical properties and efficient triplet harvesting. Building on these developments, we explore boron–nitrogen-substituted polycyclic aromatic hydrocarbons (BNPAHs) as promising candidates for fifth-generation OLEDs[1]. These next-generation materials rely on delayed fluorescence from inverted singlet and triplet states (DFIST), where the first excited singlet lies below the triplet, enabling exothermic reverse intersystem crossing. Previous DFIST studies have focused on triangular anti-aromatic cores, which often suffer from structural instability[2]. In our earlier work, we also showed that such Hund's rule-violating systems are absent in the small-molecule chemical space[3]. A recent study extended this search to heteroatom-doped PAHs and found small singlet–triplet gaps[4], though none with true inversion. In this work, we go further to systematically investigate a large aromatic space of 30,797 BNPAHs derived from 77 scaffolds. Using a multi-step workflow combining stability checks and accurate excited-state calculations, we identify 46 robust candidates with negative singlet–triplet gaps. Notably, some exhibit inversion via through-space charge transfer and feature non-planar helicenes, expanding the design space for efficient, stable, metal-free OLEDs.

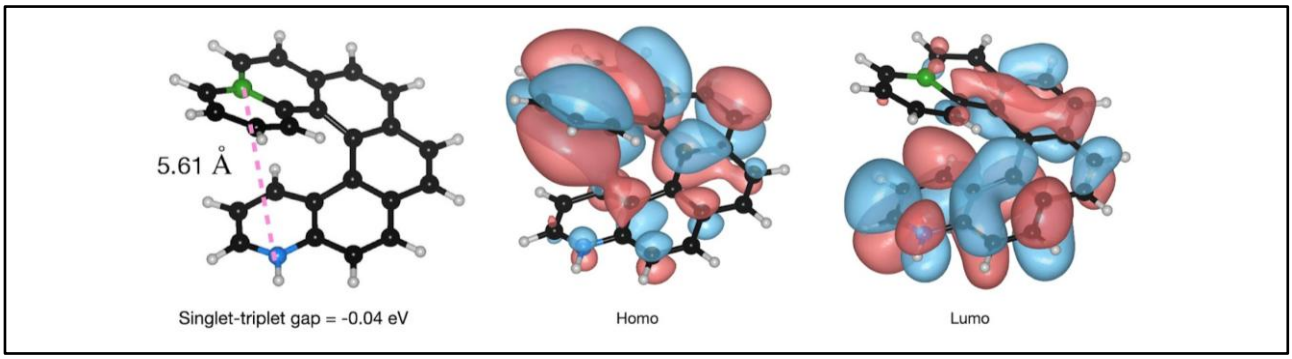


Figure 1: B,N-hexahelicene with a negative singlet-triplet gap[1]

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Influence of Vibrational Strong Coupling on Product Selectivity in Post-Transition State Bifurcation Reactions

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Vibrational strong coupling (VSC), achieved by embedding molecules in optical cavities, has emerged as a promising route to alter chemical reactivity[1]. Yet, the mechanistic origins of its mode-specific effects remain unclear. To address this, we investigate post-transition state bifurcation (PTSB) reactions, where a single transition state branches into multiple products with selectivity governed by subtle dynamical effects[2,4]. Their extreme sensitivity to perturbations makes them an ideal platform to examine how cavity–molecule interactions reshape outcomes. Using a minimal two-dimensional PTSB model with a valley–ridge inflection and asymmetric product wells, coupled to a quantized cavity mode, we observe clear signatures of control. Systematic variation of cavity frequency and barrier parameters shows that branching ratios can be modulated under VSC, with selectivity enhanced by nearly a factor of two. Although many vibrational modes are present, the cavity responds selectively to resonant ones, enabling targeted modulation of product distributions. Strikingly, classical and quantum dynamics display strong correspondence across specific regimes, underscoring the robustness of the effect. These findings highlight the dual role of cavities in redistributing energy[3] and hybridizing modes, offering a powerful handle to steer bifurcating reactions. More broadly, they suggest that VSC can be harnessed to rationally control selectivity in systems where conventional rules fail, positioning cavity quantum electrodynamics as a powerful strategy for directing dynamics across complex potential energy landscapes.

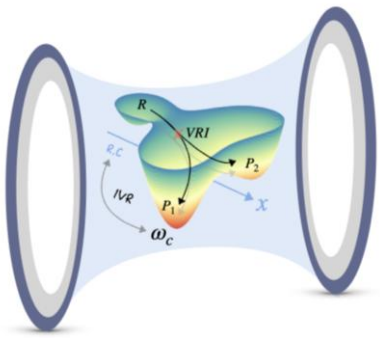


Figure 1. PTSB surface inside an optical cavity.

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Study of Photophysical properties of Phospha[5]helicene system as a function of position of phosphole ring

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This work presents a systematic investigation of the photophysical properties of phospha[5]helicenes, including absorption, excited-state geometries, spin-orbit coupling, and intersystem crossing (ISC) rates. Three pristine phospha[5]helicenes (as shown in Fig.1) with varying positions of the phosphole ring, along with their donor-acceptor substituted derivatives, were examined in the gas phase and in four different solvents using state-of-the-art TD-DFT methods. For reference, the pristine systems were further compared with their carba[5]helicene analogues. The absorption spectra of phospha[5]helicenes were found to be largely insensitive to solvent polarity and displayed a slight red shift relative to the corresponding carba[5]helicenes. Notably, relocation of the phosphole ring from the terminal to the central position of the helical backbone induced a pronounced blue shift of approximately 70 nm. In contrast, ISC rates were strongly dependent on both the position of the phosphole ring and the donor–acceptor substitution pattern. These trends are rationalized in terms of the orbital characteristics and the nature of the excited states involved.

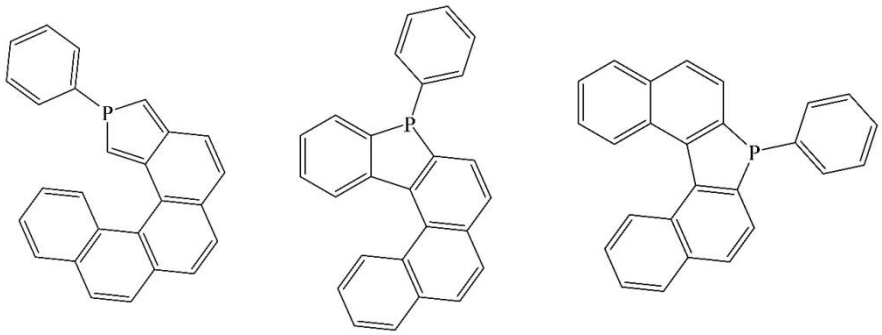


Fig. 1: Structure of three pristine Phospha[5]helicene

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Machine-Learned Insights into Solid Electrolyte Interphase Formation in Calcium Metal Batteries.

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Understanding solvation mechanisms is vital in electrochemistry, particularly for battery performance. The cation's solvation shell near the anode significantly influences solid electrolyte interphase (SEI) formation, a key factor in battery stability. Experimental techniques struggle to capture the SEI formation and evolution mechanisms non-invasively. First-principles methods like DFT, though insightful, are limited by high computational cost at larger length and timescales. In this ongoing work, we investigate the solvation shell structure and SEI formation[1] in electrolytes made of $Ca(TFSI)_2$ salt in ethylene and propylene carbonate solvents. Employing data-efficient machine-learned potentials such as DeepMD[2] and MACE[3], we overcome the computational limitations of modeling amorphous SEIs, enabling accurate electrolyte dynamics simulation to quantify reactions at the atomistic scale. Our findings provide deeper insight into ion-solvent interactions and highlight how tuning solvation shell preference potentially controls SEI formation. These insights contribute to rational electrolyte design for next-generation calcium-metal batteries.

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Evaluating eco-friendly auxin herbicide altenatives: A comparative analysis for the management of weed by Molecular Dynamics simulation

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Phytohormones or plant hormones, are mostly organic molecules that play a key role in handling numerous stress signals and overall plant growth. Auxin is one of the phytohormones that is involved in the overall development of plants, regulates plant growth, and participates in resistance to abiotic stresses. The synthetic analogs of auxin e.g. 2,4-D, NAA show toxic effects and harmful for nature and human health. So, recognition of new auxin analogs becomes important for taming this problem. In our study, we have conducted MD simulation for a comparative analysis of azelaic acid homologs that can act as eco-friendly auxin herbicide alternative for weed management. Our study reveals that the interaction between TIR1 and AUX/IAA in presence of Suberic acid is much more than the interaction in absence of ligand. Electrostatic and van der Waals contribution in the non-bonded energy calculation also reveals that interaction between AUX/IAA and TIR1 increases in presence of Suberic acid and Pimelic acid. These results will help us to find eco-friendly and less toxic auxin herbicide alternative.

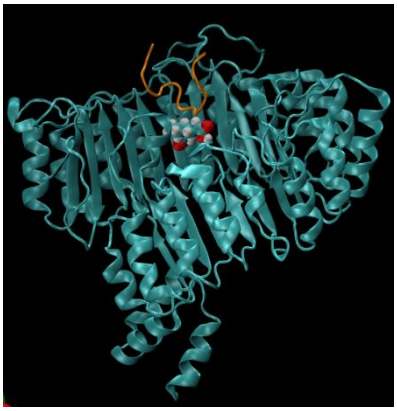


Figure: TIR1 and AUX/IAA complex in presence of Suberic Acid.

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Spin Crossover, Single-Ion Magnetism & Electron Transport in Square-Pyramidal Co(II) Complexes

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Abstract: Open-shell transition metal complexes with sizable magnetic anisotropy are highly promising towards designing new generation magnetic materials for information storage devices, qubits, and molecular spintronic applications. In this quest, Co(II) metal complexes are of special interest due to the following reasons: (i) tunable spin-states through ligand modifications, change in the coordination number;[1] (ii) The magnetic anisotropy in these systems can be directly affected by the first-order spin–orbit coupling (SOC), and (iii) the likelihood of magnetic relaxation by quantum tunneling is decreased since Co(II) is a Kramer's ion with S = 3/2. In the present work, we have thoroughly investigated the electronic structure of $[Co(3,4\text{-lutidine})_4X]^+$ (X = NCSe, SeCN, F, Cl, Br, and I) to explore how the local structural parameters and substitution control the spin-ground state in square pyramidal complexes, as the low-spin complexes show potential spin-crossover phenomena. In contrast, the high-spin complexes show potential single-ion magnet behaviour. Using relativistic density functional and multireference calculations, we shed light on electronic structure, ligand field parameters, $T_{1/2}$ values, and their correlation with 10dq and magnetic anisotropy in this family of complexes. We have also analyzed zero-field splitting parameters showing SIM behaviour. DFT+NEGF[2] calculations show that $[Co(3,4\text{-lutidine})_4Br]^+$ molecular junction exhibits NDR in the high-spin state with enhanced β-conductivity and ~99.6% spin-filtering efficiency at zero bias. Our findings highlight the dual functionality of Co(II) complexes as both SCO and SIM materials. They demonstrate their tunable electron transport behavior, providing valuable insights for designing next-generation multifunctional molecular devices.

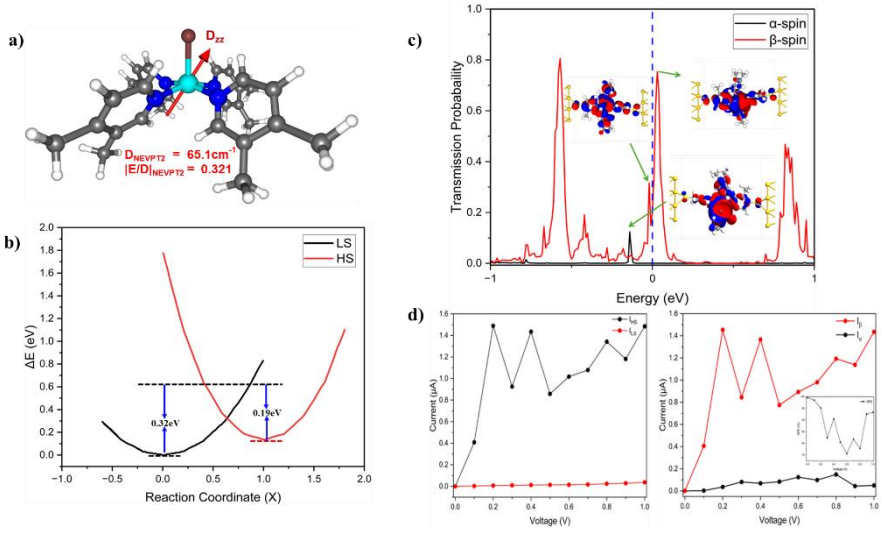


Figure 1 (a) NEVPT2 computed the orientation of the main anisotropic (D_{ZZ}) axes for $[Co(3,4\text{ lutidine})_4Br]^+$ complex; (b) Relative total energies of Co(II) SCO complexes in the HS and LS states as measured along the reaction coordinates X (c) Zero-bias transmission spectra (d) IV characteristic curve

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Catechol-O-Methyltransferase Interaction with Catecholamines and Selected Therapeutic Agents by Molecular Docking, Molecular Dynamics, and QM/MM Analysis

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Catechol-O-Methyltransferase (COMT) plays a significant role in the metabolism of catecholamines such as dopamine, norepinephrine, and epinephrine by catalyzing their O-methylation. Its role in neurochemical balance has made it an important therapeutic target for neurological and psychiatric disorders, including Parkinson's disease, schizophrenia, and depression. In this study, an integrated computational approach combining molecular docking, molecular dynamics (MD) simulations, and quantum mechanics/molecular mechanics (QM/MM) methods is employed to investigate the interaction of COMT with both its endogenous catecholamine substrates and selected drug molecules. Molecular docking is used to predict the binding orientations and affinities within the COMT active site, followed by MD simulations to assess the stability and dynamic behaviour of enzyme-ligand complexes under physiological conditions. Subsequently, QM/MM calculations are carried out to model the enzymatic methyl transfer reaction at an atomic level, providing mechanistic insights into the role of key active-site residues and the transition state stabilization. The results elucidate critical interaction patterns and energetic profiles underlying substrate recognition and inhibitor binding, offering a detailed understanding of COMT's catalytic mechanism. This multi-scale computational study enhances our molecular-level insight into COMT function and lays the groundwork for the rational design of more effective and selective COMT inhibitors.

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Tuning Hot Carrier Dynamics in Vacancy-Ordered Halide Perovskites through Lattice Compression: Insight from ab Initio Quantum Dynamics and Machine Learning

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The efficient harvesting of hot carriers (HCs) from high-energy photons can significantly enhance the optoelectronic performances. However, ultrafast HC cooling through intraband transitions poses a significant challenge for extraction using traditional semiconductor absorbers. The stable and compressible vacancy-ordered halide perovskites with isolated octahedra exhibit discrete electronic states at the conduction band edge, indicating the possible slow cooling of hot electrons (HEs). Using state-of-the-art ab initio quantum dynamics simulations and unsupervised machine learning (ML), we investigate the effect of lattice stress on HE dynamics in vacancy-ordered Cs_2SnBr_6. The moderate stress enhances structural rigidity and weakens dynamic electron−phonon interactions at the conduction bands. Such modifications and the widened energy gap at the conduction band edge partially suppress intraband nonadiabatic transitions, eventually elongating the HE lifetime. The pairwise mutual information extracts hard-to-find highly nonlinear dynamic structure-excited state property correlations, offering the unique opportunity to design efficient lead-free halide perovskites for HE-based optoelectronics strategically.

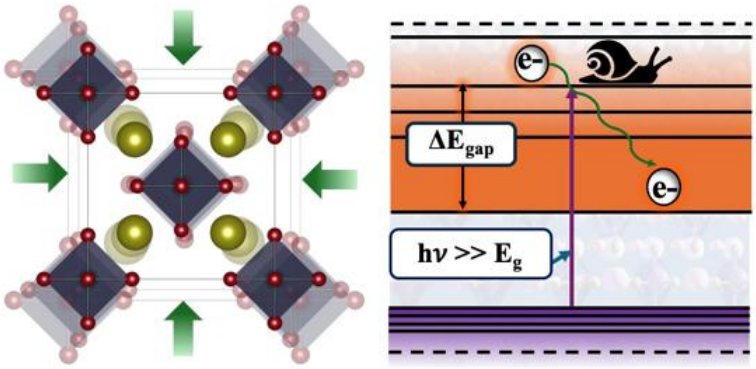


Figure 1: Hot carrier cooling in Vacancy-Ordered halide perovskite through lattice compression.

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Metal-Center Effects in MC_2N_2 Single-Atom Catalysts for Li-O_2 Batteries

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The lithium-oxygen (Li-O_2) battery is recognised as a next-generation energy storage technology owing to its exceptionally high theoretical energy density.[1] However, its practical realization is limited by sluggish oxygen electrochemistry and large overpotentials. Developing efficient and tunable electrocatalysts is essential to achieving reversible and high-efficiency Li-O_2 chemistry.[2]

In this work, we systematically investigate a series of MC_2N_2 single-atom catalysts (SACs), where the transition metal is coordinated by two carbon and two nitrogen atoms. These SACs uniquely integrate atomic-level metal utilization with well-defined and tunable coordination environments. Using density functional theory calculations, we explore how the metal center modulates oxygen binding and the energetics of lithium-oxygen intermediates. Distinct trends in adsorption strength are observed across different metals and are correlated with their electronic characteristics. Furthermore, the equilibrium potential and overpotential strongly depend on the adsorption energies of key lithium-oxygen intermediates. It highlights that the optimal balance between adsorption strength and intermediate stabilization is critical for minimizing the overpotential.

These insights emphasize the crucial role of metal-centered electronic structure in controlling oxygen electrochemistry and provide guiding principles for developing efficient cathode catalysts for Li-O_2 batteries.

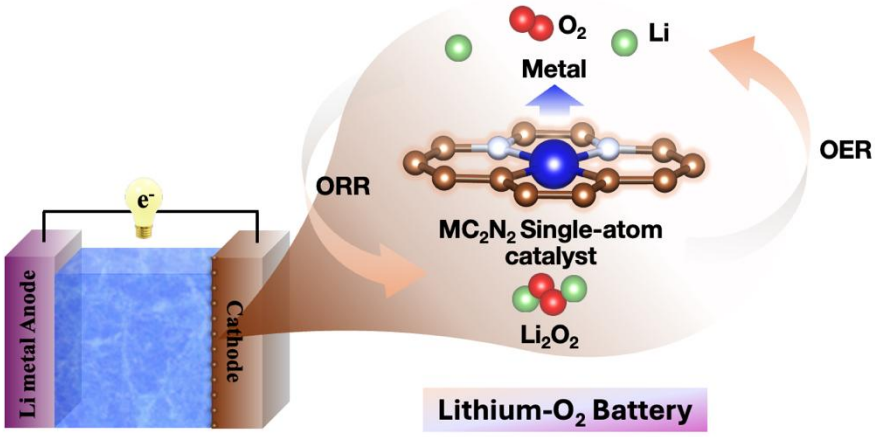


Figure 1 Graphical representation of the transition metal-substituted MC_2N_2 single-atom catalyst driving oxygen reduction and evolution reactions (ORR and OER) for Li-O_2 batteries.

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Theoretical Chemistry Symposium
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Atomistic details on the glycosylation of a peptide

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Abstract

Glycosylation significantly influences the properties and functions of peptides by attaching carbohydrate groups to specific amino acids. This modification can enhance peptide stability, solubility, and resistance to enzymatic degradation, while also affecting folding and overall structure.[1] There are some contradictory studies suggesting that glycation can enhance peptide–peptide association enthalpy, reduce conformational entropy, and promote β-sheet-rich aggregate formation.[2] Driven by such evidence, we performed atomistic MD simulations of a number of peptides derived from the A chain of human insulin, which has been shown to self-assemble. The peptides were glycosylated at different positions as per the suitable sites available. Our study inferred that the interaction between the hydrophobic residues plays a vital role in the aggregation process, as the unglycosylated peptide formed a substantially higher number of hydrophobic contacts, resulting in reduced solvent exposure over time. In contrast, glycosylation decreased the number of such contacts, consistent with reduced aggregation propensity. The Free Energy Landscape displayed two distinct minima separated by an energy barrier, indicating the presence of multiple metastable conformational states associated with aggregation. The mono-glycosylated form showed a slight shift in the primary minimum, whereas the di-glycosylated peptide exhibited a single, well-defined minimum, reflecting a simpler and less aggregation-prone conformational ensemble. Glycosylation also influenced peptide translational mobility. Diffusion coefficient indicated nearly a two-fold increase in peptide mobility upon glycosylation. These findings provide molecular-level insights into how glycosylation modulates peptide functional properties, offering a potential design strategy for reducing aggregation in therapeutic peptides through glycosylation.[3]

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Investigating the Role of Various Substitution Strategies in Cs_2AgBiI_6 Double Perovskite Toward the Enhancement of Its Optoelectronic Properties

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Our first-principles calculations reveal how Cu and Na substitution modify the structural, electronic, and optical properties of Cs_2AgBiI_6 halide double perovskite (HDP). Cu doping significantly reduces the band gap and enhances light absorption across the UV-visible and near-infrared regions, with optimal effects at 25–75% substitution. Na doping induces minor band dispersion and optical changes. Doping-dependent shifts and intensification in absorption peaks underscore the potential of tailored HDPs for optoelectronic applications, especially in photovoltaic and photodetector technologies.

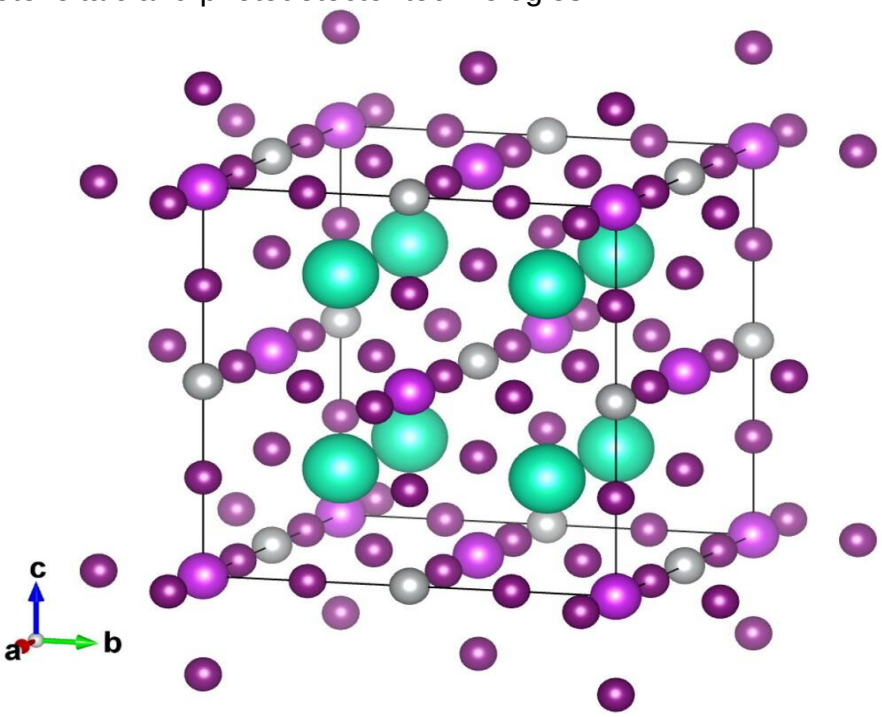


Figure 1: Optimized geometry of Cs_2AgBiI_6 double perovskite. Atoms are colored as follows: Cs - teal, Ag - gray, Bi - light purple, and I - purple.

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Machine Learning of Thermodynamic Ergotropy in Cavity-Mediated Quantum Batteries

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Abstract

Optimizing quantum-battery performance that leverages through quantum coherences and depend upon parameter optimisation and thermodynamic quantities like ergotropy (ε), proves challenging in open systems where populations and coherences are intrinsically coupled. Here, we study a four-level cavity-mediated quantum battery using quantum master equations combined with hybrid machine learning to identify optimal operating regimes. Feature importance analysis followed by testing revealed a minimal four-parameter subset-kurtosis $C^{(4)}$, cold bath coherence strength (p_c), temperature of the hot reservoir (T_h), and heat input (Q_h) that attains an accuracy of 0.90. Expanding to eight parameters by adding heat output (Q_c), leak reservoir temperature (T_l), first excited state energy (ε_b), and second excited state energy (ε_a) yielded an accuracy of 0.98. The four-parameter option offers practical advantages, since collecting four measurements is significantly easier than obtaining eight distinct parameters in experimental or computational quantum battery systems. These results indicate that path-induced coherences can enhance work extraction beyond classical limits and offer flexibility between minimal and comprehensive protocols for quantum energy storage optimization.

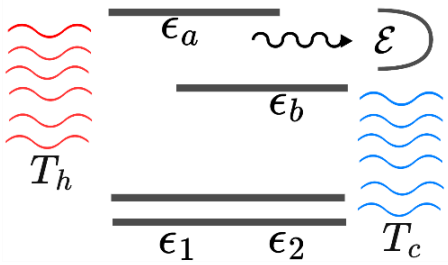


Figure 1. Schematic representations of the quantum-battery model showing coupling to hot and cold reservoirs.

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Designing Fold-Switching Proteins using Cα-based Statistical Potential

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Computational methods have been applied to design and redesign protein sequences that fold to a single ordered and stable state, the computational design of protein sequences with high sequence similarity that adopt well-defined but structurally divergent structures remains an outstanding challenge. We designed 28 pairs of sequences using Monte Carlo simulation, denoted as (a_1, b_1), (a_2, b_2), (a_3, b_3), ..., (a_{28}, b_{28}), where a_i and b_i represent sequences adopting the 3-α fold and 4β + α fold, respectively. Among these, we identified three sets of fold-switching protein sequences, (a_1, b_1), (a_2, b_2) and (a_3, b_3): one with 89.29% sequence similarity and two others with 87.50% sequence similarity. This reflects the ability of statistical potential to finely balance competing structural constraints. The designed sequences differ by only few residues; however, they possess different tertiary structures: a 3-α helix fold and a 4β + α fold. In addition, sequence variants for a_1, a_2, and a_3 are also designed using rational design guided by sequence analysis, and the results show striking outcomes: single point mutations, specifically D26C or A39F in a_1, are sufficient to induce fold switching from the 3-α fold to the 4β + α fold while maintaining 98% sequence similarity with the parent sequence. Together, these findings suggest that the design approach is successful in designing fold-switching sequences that are compatible with their respective target structures. This work also ensures that the developed one-body and two-body statistical potentials are successful in designing protein sequences that exhibit fold conservation and the fold-switching phenomenon, as well as stability at the respective target structures.

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Leveraging Machine Learning to Predict Photophysical Properties of Squaraine Dyes

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Squaraine dyes constitute an important class of organic chromophores with applications in dye-sensitized solar cells, photodynamic therapy, bioimaging, and chemical sensing[1]. Understanding their photophysical properties is crucial in assessing its potential applications[2]. The traditional synthetic pathway is usually slow, resource-intensive, and involve ad-hoc procedures[3]. A priori knowledge of the dye profile will greatly benefit the scientific community which can be achieved utilizing the data-driven Machine Learning (ML) approaches. In this study, we have attempted to apply the ML techniques to predict the photophysical properties of squaraine dyes[4]. A dataset of squaraine dyes is curated, molecular descriptors together with solvent related features are generated and refined for analysis. Machine learning models are developed and evaluated using standard statistical metrics (R^2, MAE, RMSE) to predict photophysical properties under different solvent conditions. Models are systematically compared, and the selected ones exhibit strong correlation, highlighting their predictive power on novel molecules.

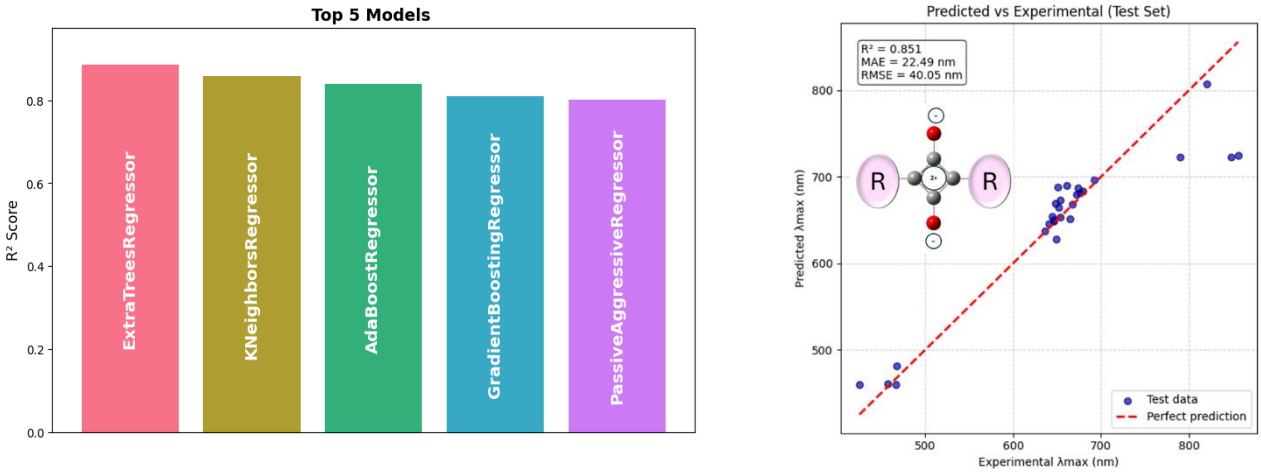


Figure 1. A comparative performance plot of the ML models with the highest R^2 score and the scatter plot of the λ_{max} values using *Extratreesregressor*. The structure of the squaraine dye is given in the inset.

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Theoretical Chemistry Symposium
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In silico Insights into the Binding and Inhibition of Acetylcholinesterase 1 (AChE1) from *Rhipicephalus microplus*

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Acetylcholinestearase is an important neurotransmitter regulating enzyme and potential target for managing *Rhipicephalus microplus.* This study analyses the binding and inhibitory potential of plant derived terpenoids 1,8-cineole and Linalool compared to synthetic Diethyltoluamide (DEET) using molecular docking and molecular dynamic approaches. The study show that these compounds bind stably on the predicted catalytic triad residues (Glu255, Ser256, His494) which directly involves in acetylcholine hydrolysis, which lead to competitive inhibition. The compounds showing binding site occupancy through molecular docking and stable binding through MM-PBSA strongly suggests they can physicially and chemically block substrate access and catalytic function. It is evident that 1,8-cineole and Linalool have potential as AChE1 inhibitors for management of *R. microplus* ticks as they show stronger MM-PBSA binding than the known inhibitor DEET.

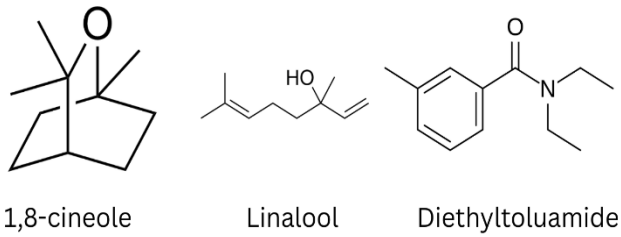


Figure 1: Structure of Compounds

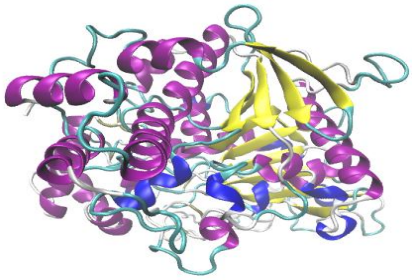


Figure 2: Structure of AChE1

Compound	Docking Score	MM-PBSA (ΔG)
Linalool	-5.773 kcal/mol	-4.2792 kcal/mol
1,8-cineole	-6.522 kcal/mol	-4.0570 kcal/mol
DEET	-7.295 kcal/mol	-3.9171 kcal/mol

Table 1: Binding affinity

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Theoretical Chemistry Symposium
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Molecular Insights into the Role of Heteroatoms on the Thermal and Rheological Behaviour of Asphalt Binders

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Abstract

Asphalt binders play a central role in road infrastructure, and their performance is heavily influenced by both their chemical composition and their response to temperature changes [1,2,3]. In this study, we used all-atom molecular dynamics simulations to explore how variations in chemical structure, particularly the presence of heteroatoms such as oxygen, nitrogen, and sulfur, affect the behavior of asphalt at the molecular level. We designed a set of surrogate asphalt models based on realistic SARA fractions, including a baseline model and six modified versions with elevated heteroatom content. Among these, the AM-3O, AM-3N, and AM-3S models were selected for detailed analysis, as their densities closely match those typically reported in experiments. By simulating these models across a wide temperature range (100 K to 533.15 K), we captured important thermal and physical trends, including changes in density, volume, diffusivity, and viscosity. The three systems transitioned through different mechanical states, from glassy to viscoelastic to Newtonian fluid, with glass transition temperatures (Tg) clustered around 265–273 K. Although heteroatom content and type affect overall density, they had only a modest effect on Tg and viscoelastic-to-Newtonian fluid transition temperatures (T_X). These insights reveal how subtle changes in molecular structure can influence the flow and performance of asphalt binders, providing useful guidance to tailor materials to with stand environmental and mechanical stress better.

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Molecular Mechanism of Stilbenoids Disruption Potential on Aβ42 Protofibril

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Amyloid-β42 (Aβ42) aggregation into protofibrils drives Alzheimer's disease (AD) pathology, making their disruption a key therapeutic strategy. We investigated five biphenolic stilbenoids—Resveratrol, Piceid, Astringin, Piceatannol, and Rhapontigenin—using docking, 500 ns molecular dynamics, MM-PBSA, and structural analyses (RMSD, RMSF, Rg, hydrogen-bond/salt-bridge dynamics, intersheet contacts, and PCA). All ligands bound β-sheet hotspots (Phe19, Phe20, Val36, Gly38). Rhapontigenin was most potent (ΔGbfe = −16.7 ± 5.8 kcal/mol), disrupting hydrogen bonds, salt bridges, compactness, and inducing chain-terminal deformation and conformational broadening. Piceatannol and Piceid showed moderate effects, while Astringin and Resveratrol were weaker. Rhapontigenin emerges as a strong scaffold for anti-amyloid therapeutics.

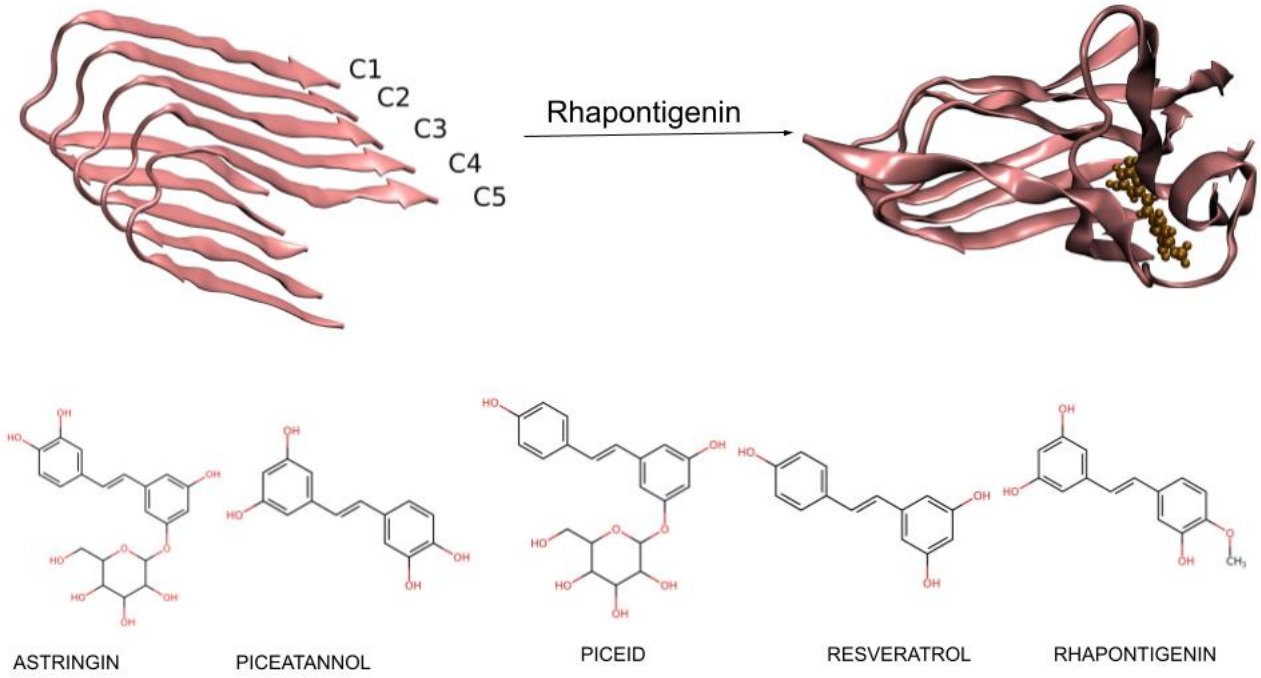


Figure: Snapshots of the configuration correspond to Aβ42 - Protofibril (2BEG) in the presence of Rhapontigenin at the beginning and at the end of the 600ns simulation. Thechemical structure of Astringin, Piceatannol, Piceid and Resveratrol are also incorporated. .

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Theoretical investigation on the scavenging mechanism and kinetics of hydrazone compounds towards hydroperoxyl and methylperoxyl radicals.

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Abstract: Herein**,** a comprehensive density functional theory (DFT) investigation was conducted to examine the scavenging activity of six heterocyclic hydrazone derivatives (Figure 1) against the reactive oxygen species. Three reaction mechanisms were investigated: hydrogen atom transfer (HAT), single electron transfer proton transfer (SETPT), and sequential proton loss electron transfer (SPLET). These mechanisms were evaluated based on thermodynamic parameters, including bond dissociation enthalpy (BDE), ionization potential (IP), proton dissociation enthalpy (PDE), proton affinity (PA), and electron transfer enthalpy (ETE) in different media, namely the gas phase, water, and pentyl ethanoate.[1] Among the studied compounds, compound 2 exhibited the highest reactivity toward HOO• scavenging via the HAT mechanism in the gas phase at the O2′-H site. For CH_3OO• scavenging, it showed the most pronounced activity at the N8-H and O2′-H sites. The results suggest that compound 2 shows antioxidant activities comparable to butylated hydroxyanisole consistent with experimental findings[2], representing its potential as an effective scavenger of hydroperoxyl and methoxy peroxyl radicals. The anionic form of compound 2 showed the greatest HOO• and CH_3OO• radical scavenging activity among all of the studied compounds with rate constants of k_{app} = 1.8 × 10^7 M^{-1} s^{-1} and k_{app} = 3.3 × 10^6 M^{-1} s^{-1}, respectively in water solvent.

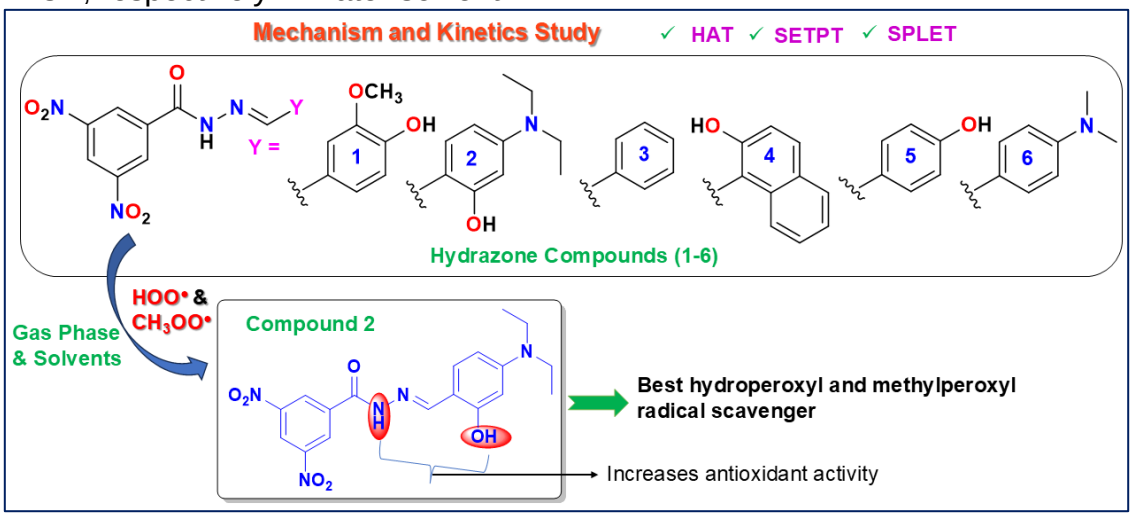


Figure 1 Six hydrazone compounds as potent hydroperoxyl and methyl peroxyl radical scavengers.

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Predicting oral bioavailability of cyclic peptide therapeutics using physics-based modeling

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Peptides are quickly becoming an attractive option for the discovery of novel therapeutics due to their unique properties. Peptide drugs combine the advantages of antibodies including high binding affinity, target specificity and the potential to bind surfaces that have traditionally been undruggable, with those of small molecules such as oral bioavailability. In particular, cyclic peptides (CPs) have become popular due to their increased stability towards enzymatic degradation. However, predicting the oral bioavailability of CPs poses a significant challenge owing to their flexibility, notwithstanding the partial rigidification of the peptide conformation caused by cyclization. Here we describe enhancements to the Schrödinger computational platform facilitating *in silico* prediction of membrane permeability of CPs, a quantity that is correlated with bioavailability of oral drugs. In particular, we present a physics-based protocol for determining the transfer free energy of cyclic peptides, calculated as the difference in single-point energies in high (water-like) and low (lipid-like) dielectric environments. Our method is validated against multiple publicly available data sets and different *in vitro* assays.

Hybrid RNN–Fingerprint Models for Yield Prediction in Transition Metal-Catalyzed Cross-Coupling Reactions

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Machine learning is revolutionizing chemical research by enabling fast and accurate prediction of reaction outcomes. In this study, we developed hybrid recurrent neural network–fingerprint (RNN–FP) models to predict the yields of transition metal-catalyzed cross-coupling reactions using a dataset of about 4,901 reactions catalyzed by palladium, nickel, copper, cobalt, iron, zinc, and manganese, divided into training, validation, and test sets in a 70:10:20 ratio. The hybrid framework integrates RNN architectures—LSTM, GRU, BiLSTM, and BiGRU—with Morgan fingerprints to capture both sequential (SMILES) and structural molecular features. Among all variants, the BiLSTM–Fingerprint (BLF) model achieved the best performance, with an R^2 of 0.83 on a random test split and 0.94 on a custom test set of palladium-catalyzed reactions. Standalone RNNs without fingerprint features yielded lower R^2 values (0.64–0.67), confirming the advantage of combining structural information. Overall, this hybrid deep learning approach demonstrates enhanced accuracy and generalization in data-scarce and chemically diverse reaction spaces, offering a reliable tool for catalyst-specific yield prediction and reaction optimization.

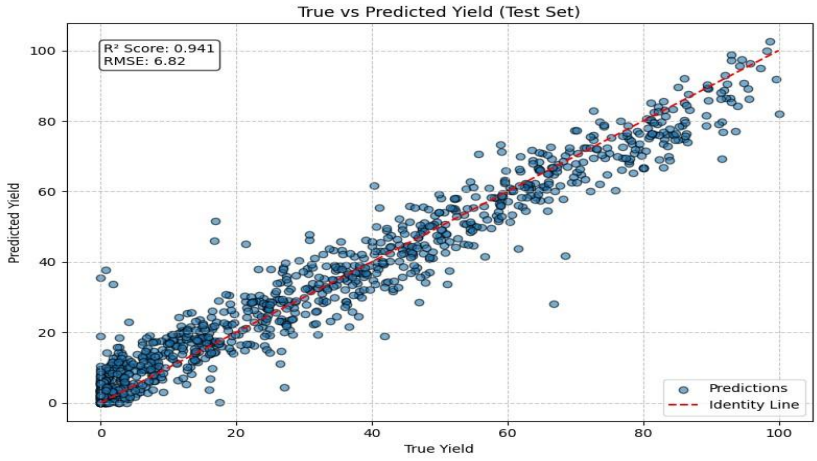


Figure 1 : *True vs. predicted reaction yields obtained using the BiLSTM–Fingerprint (BLF) model on the test set, showing an excellent correlation (R^2 = 0.941, RMSE = 6.82) between predicted and experimental values.*

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Study of neutralization of O^+ through charge transfer: An application to supernova spectral modelling

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The importance of charge transfer (CT) processes in the supernova (SN) has long been recognized and well studied.[1] A detailed study of such processes is conducted through spectral analysis, which requires cross sections and rate coefficients.[2,3] These are obtained from dynamic calculations on the accurate potential energy surface and couplings among them, such as radial, rotational, and spin-orbit interactions. The neutralization of O^+ through CT reaction, $C + O^+ \rightarrow C^+ + O$ (^1D) has been observed in SN ejecta.[2] We studied 32 low-lying electronic states for the CO^+ molecular ion, focusing on the entrance and CT channel, and non-adiabatic interactions among them. The cross section is calculated using quantum mechanics[3] on the diabatic potential energy curves (PEC) (See Figure 1(a, b)). The rate coefficients are found to play a crucial role in determining the strength of the [OI] doublet at 6300 and 6364 Å in the SN ejecta.

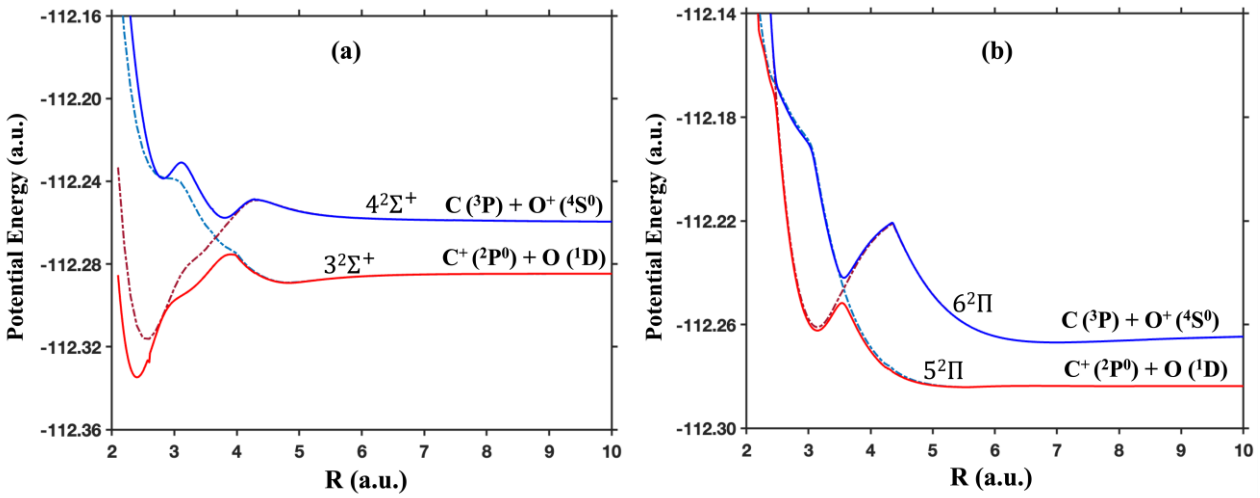


Figure 1 Adiabatic (solid lines) and diabatic (dash-dotted lines) PECs of (a) $3^2\Sigma^+$ and $4^2\Sigma^+$ (b) $5^2\Pi$ and $6^2\Pi$, of the CO+ molecular ion as a function of internuclear distance R.

We further extend our study to the neutralization of O^+ ions in collisions with the abundant species S, Si, Ne, and Mg found in SN ejecta.[2,4]

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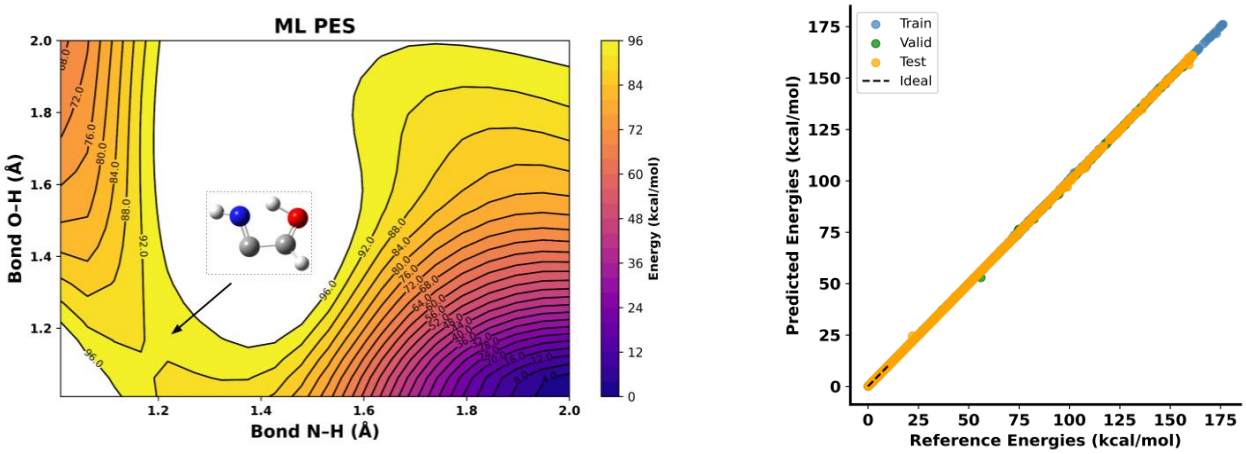
Computational Investigation of Glycolonitrile Formation in the Interstellar Medium

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Glycolonitrile ($HOCH_2CN$), the simplest cyanohydrin, is a key precursor to prebiotic compounds such as **adenine [1]**. It was first detected in the **interstellar medium (ISM)** in 2019 [2]. Previous **quantum-chemical calculations** have proposed multiple formation pathways for glycolonitrile using the **AutoMeKin** software [3]. In this work, the **reaction dynamics** of one selected pathway, in which formyl radical (**HCO)** and amino-carbyne radical (**H_2NC)** both species were known to exist in the ISM, react to form glycolonitrile via a **proton transfer mechanism**. A **dataset** was first generated using Density Functional Theory (DFT) with ωB97XD in combination with Def2-TZVPP basis set, and a **global potential energy surface (PES)** was constructed using the (**MACE) framework [4],** a machine learning interatomic potential method. This PES captures the entire reaction coordinate, including proton transfer steps leading to glycolonitrile formation. M**olecular collisions** were simulated on the PES to investigate the **reaction pathways and dynamical effects**. In addition, **collision dynamics** between reactants were also examined to characterize product formation in both the **reactant** and **product channels**.



(a) (b)

(a) Contour diagram of the potential energy surface showing proton transfer from N–H to O, with the corresponding transition state (TS) shown in the inset. (b) Correlation plot of ML predicted Vs reference potential energies.

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POTENTIAL-DRIVEN INTERFACE REORGANIZATION CONTROLS PROTON TRANSFER IN NITROGEN REDUCTION REACTION

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Electrocatalytic nitrogen reduction reaction (NRR) is a sustainable alternative pathway for NH_3 synthesis, but inhibiting the competing hydrogen evolution reaction (HER) remains challenging. The Catalyst activity can be tuned by adjusting the applied electrode potential, which not only governs reaction kinetics but also reorganizes the electric double layer (EDL) at the electrode-electrolyte interface[1], which remains unexplored. We employ constant-potential ab *initio* molecular dynamics (AIMD) simulations[2] to investigate the effect of applied potential (0, -0.2, and -0.4 V vs RHE) on the interfacial microenvironment in an acidic medium at the MoN_4/H_2O electrochemical interface. The interfacial microenvironment is analyzed using the water density profile, water orientation angle ($\cos \phi$), and the H-bond network along the surface. Our simulations reveal that, at lower potentials, water molecules are disordered, forming a disrupted H-bond network. However, more negative potentials enhance the ordering of water molecules, forming a dense H-bond network that facilitates efficient proton transfer. Consistently, the $*NH_2$ to $*NH_3$ transition is a potential-determining step of NRR, and the slow growth simulation suggests that as the potential becomes more negative, the reaction barrier of $*NH_3$ decreases from 0.559 eV (0 V) to 0.421 eV (-0.4 V). Furthermore, the oxophilic behavior of Mo is responsible for reorganizing the interfacial water molecules, directly influencing the HER. In HER, proton transfer is coupled with an electron, approximately 0.734 |*e*|, close to 1 |*e*|. It is noteworthy that catalytic activity depends solely on the reaction environment, specifically the interfacial environment near the electrode. This study provides key insights into the potential-dependent EDL modulation of NRR and offers a strategic foundation for designing electrocatalysts and electrolyte systems for efficient ammonia production.

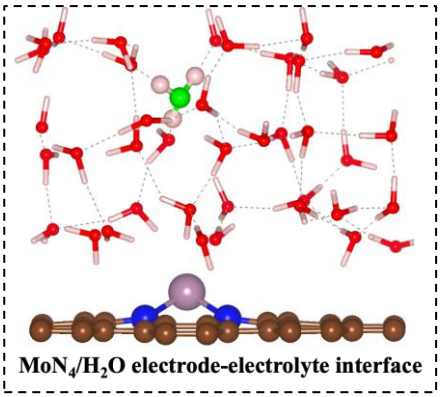


Figure 1: The representative snapshots of the MoN_4/H_2O electrochemical interface

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Mechanistic Exploration of the Ligand free Nickel catalyzed Suzuki–Miyaura Coupling Reaction : A DFT Study

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The Suzuki–Miyaura reaction is a widely used method for C–C bond formation in pharmaceuticals, agrochemicals, and materials. While palladium catalysts are efficient, their high cost and sustainability issues limit large-scale use. Nickel offers a low-cost, abundant alternative, and ligand-free systems further enhance practicality by avoiding expensive or air-sensitive ligands. However, a lack of mechanistic understanding has hindered the effective utilization of these catalysts.In this study, the mechanism of ligand-free nickel-catalyzed Suzuki coupling was investigated for the first time using Density Functional Theory (B3LYP) on a model system comprising 4-bromoanisole and phenylboronic acid with K_3PO_4 in 1,4-dioxane. In contrarst to the conventional Palladium mechanism, computed results reveal that nickel catalyzed Suzuki coupling reaction is more likely to proceed through an initial transmetalation step, which is also the rate determining step. This study unveils new mechanistic insight into nickel catalysis, wherein inexpensive and readily available $NiCl_2 \cdot 6H_2O$ facilitates ligand- and reductant-free coupling of aryl bromides and iodides, highlighting a practical and sustainable catalytic system.

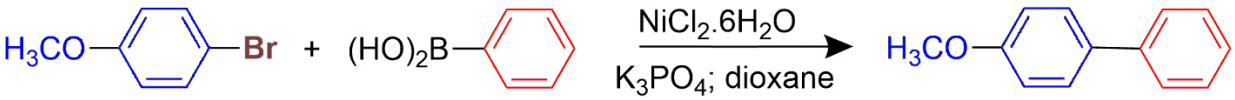


Figure 1 Model Reaction Mechanism for Ligand free Nickel- Catalyzed Suzuki-Miyaura Coupling.

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Ab Initio Study of Photoisomerization in Styrylpyridines: Positional Effects in 2-, 3- and 4-Isomers

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The intersection of photochemistry and material science has propelled a dynamic research frontier focused on photochromic molecular switches and memories,[1,2] where precise control of molecular structures gives rise to tunable material functionalities. Photochromic compounds such as azobenzene[3] and stilbene[4] exhibit reversible isomerization and color changes upon irradiation, accompanied by shifts in geometry, quantum yield, and absorption spectra[5]. This controlled switching enables the selective activation and deactivation of photoswitches[2] and tailored responses in photomemories[6]. Such light-driven reversibility are essential for unlocking new possibilities in the development of innovative materials with potentially improved electro-optical properties.

Building upon these foundations, we present a detailed theoretical analysis of the photoinduced isomerization and cyclization pathways in 2-, 3- and 4-styrylpyridine (STPY) isomers, motivated by their potential for precise photocontrol at the molecular level. Using MP2 and ADC(2) methods, we systematically explored their conformational energy landscapes and excited-state properties to understand how structural variations govern their photochemical behavior. The position of the pyridine nitrogen atom was found to play a central role in modulating their photodynamics: 2- and 3-STPY exhibit multiple accessible rotamers and significant conformational flexibility, while 4-STPY shows limited conformational flexibility, yielding only a single isomer per configuration. To probe the non-radiative decay mechanisms following photoexcitation, minimum energy conical intersections (MECIs) between the S_0 and S_1 states were located using the CASSCF method. The comparative analysis of these STPYs indicates that the nitrogen atom's position strongly influences the potential energy surface topology, resulting in different deactivation and reaction pathways. These distinctions are attributed to differences in electronic distribution and steric constraints imposed by the substitution pattern. The findings offer mechanistic insight into the excited-state processes in styrylpyridine derivatives and suggest isomer-specific pathways for photoinduced isomerization and cyclization of the molecules.

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State-to-State Transport Analysis: Unraveling Quantum Pathways in Molecular Aggregates

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Transport in molecular aggregates—whether of excitations, charges, or other quantum particles—can proceed along multiple competing pathways, each shaped by distinct pumps, drains and transport efficiency moderated by the thermal environment. While on-site populations might give an inkling of the pathway, in most real-world transport systems like photosynthetic light harvesting complexes and molecular wires, it is insufficient and lacks mathematical rigour.

We present the recently developed **state-to-state transport analysis**[1], which decomposes system dynamics into direct, time-resolved, unmediated flows between pairs of sites while fully incorporating environmental effects. This framework enables the reconstruction of transport pathways from the pairwise flows. A **non-Hermitian extension**[2] of this method can account for multiple sinks, yielding sink-resolved transport efficiencies while a more recent **Lindblad state-to-state formulation**[3] expands the scope further, incorporating pumps, dephasing, and arbitrary processes described by Lindblad operators.

We demonstrate these methods on excitonic and polaritonic systems, both with and without external pumps and drains. Importantly, our framework is simulation-agnostic, compatible with semiclassical, perturbative, and numerically exact techniques. Altogether, state-to-state analysis offers a rigorous and intuitive means of uncovering transport mechanisms in complex quantum systems, with direct implications for the design of materials optimized for quantum transport.

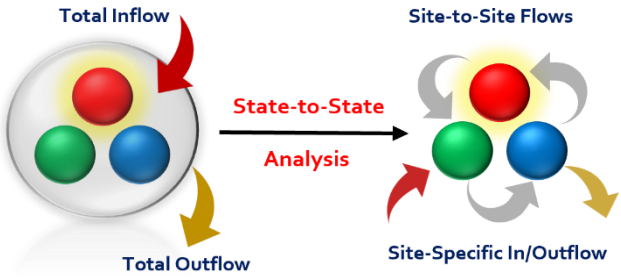


Figure A schematic describing State-to-State Transport Analysis

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Unveiling the Origins of Life: Gas-Phase Mechanisms for Interstellar Amino Acid Formation

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The origin of life on Earth remains an unresolved question that continues to attract significant scientific interest. Early experiments by Urey and Miller demonstrated the abiotic formation of amino acids under simulated prebiotic conditions, highlighting their central role as the building blocks of proteins. The detection of amino acids such as glycine, along with their precursors, in the interstellar medium has further raised the possibility of amino acid synthesis beyond Earth. In this study, the potential formation of chiral amino acids in the interstellar medium is explored through gas-phase reactions. Experimentally detected small organic molecules are considered as precursors for alanine formation. Two mechanistic pathways are proposed, both initiated by the methyl radical, cyanide radical, carbon monoxide radical, and water, involving radical–radical and radical–neutral interactions. Quantum chemical methods were employed to investigate the reaction mechanisms. The calculated reaction energies, potential barriers, and optimized geometries suggest that the proposed pathways for alanine formation are energetically feasible.

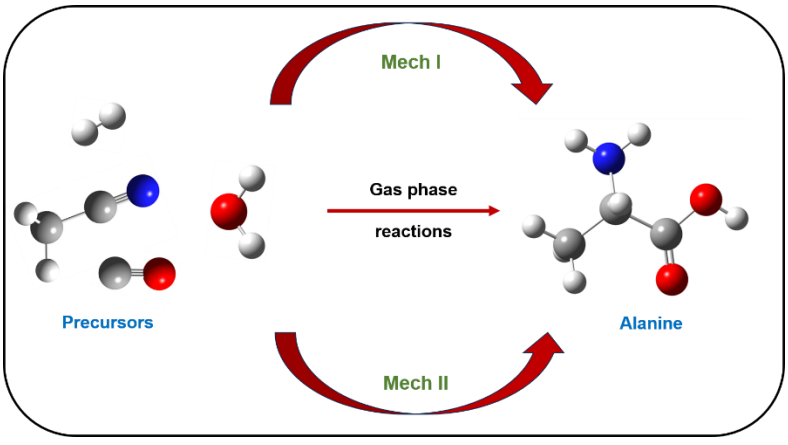


Figure 1: Graphical representation of amino acid formation

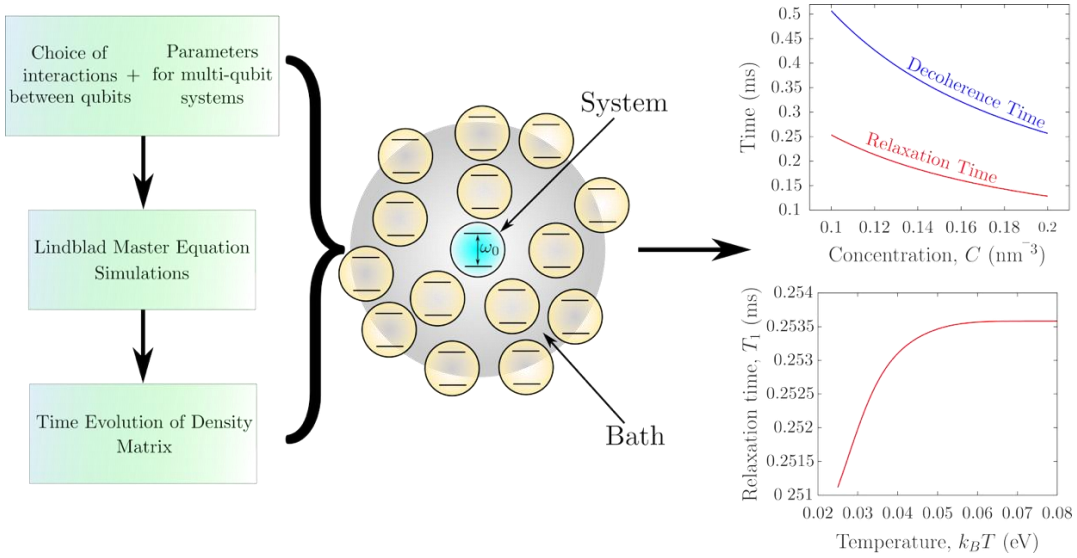
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Analyzing Decoherence in Multi-Qubit System Using Mean-Field-Based Lindblad Master Equation

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Multi-qubit systems offer a promising role for scalable quantum technologies, enabling fault-tolerant computing, faster error correction, and advanced algorithms. However, their performance is limited by strong decoherence due to environmental noise and qubit–qubit interactions. Extensive research is ongoing to investigate fidelity of multi-qubit gates [1], concurrence of multi-qubit states [2], and environmental effects on single qubits [3], however, it is still unclear how interactions between qubits, their concentration, spatial distributions, or temperature of the bath affect qubit relaxation and dephasing times. To address this gap, we have developed an analytical framework that analyzes the population dynamics of energy levels and the quantum coherence of a given solid-state qubit interacting with other qubits in a multi-qubit system. Our framework uses the Lindblad master equation approach and includes the inter-qubit interactions within a mean-field approximation. By explicitly incorporating qubit–qubit interactions, we can examine how qubit characteristics such as energy level differences, critical interaction distances, and types of interactions affect the qubit dynamics. Our analysis reveals that increasing the concentration of qubits leads to shorter relaxation and decoherence times. The model successfully explains recent experimental observations in Er^{3+}doped CeO_2, where relaxation times are reported to decrease with increasing dopant concentration [4]. We also observe that qubit relaxation slows down at elevated temperatures, while decoherence is accelerated. Our framework offers a novel approach to exploring multi-qubit system behavior by explicitly incorporating qubit–qubit interactions and supporting the design of qubits that can maintain coherence under real-world conditions.



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Facet Engineering in Halide Perovskite Nanocrystals for Modulating Energy Level Alignment and Emission Behavior

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Halide perovskite nanocrystals (HPNs) have emerged as promising avenue for optoelectronics due to their near-unity photoluminescence quantum yield (PLQY), high defect tolerance, and tunable emission properties. Facet engineering of such nanocrystals (NCs) offer significant opportunities for optimizing their energetic and electronic behaviors. However, due to the uneven distribution of surface electrostatic potentials at undercoordinated sites makes it challenging to model the faceted NC and hence to establish an atomistic understanding on the structure property correlation between faceted NCs and their optoelectronic properties. In this work, using state-of-the-art level of electronic structure calculations, we have systematically investigated the role of facet engineering on energy level alignment and emission behavior of $CsPbBr_3$ NCs with a vis-a-vis comparison with the surface slabs in order to reveal the importance of the consideration of realistic model in studying HPNs and establishing a structure-property correlations upon facet truncation. We have found that, for the almost similar sized NCs, the work function can be tuned up to 2.20 eV with a proper faceting compared to that of slabs, where it can be tuned up to 1.42 eV. We observe a notable variation in the excited states energetics and emission behavior upon facet tuning, showing a STE to non-STE like electron-hole (e-h) pair formation upon introducing 110-facets into the 100-facet based hexahedron NC, thus showing more non radiative recombination in highly faceted cuboctahedra or decahedra NC compared to that of less faceted hexahedron shape. Such modulation of energy level and emission behavior originates from the different extent of unsaturation of the facets of the NCs. This study offers the comprehensive understanding of facet engineering in HPNs for an effective design strategy in tuning the electronic and optical behaviour of HPNs, thereby tailoring them into a wide range of optoelectronic applications.

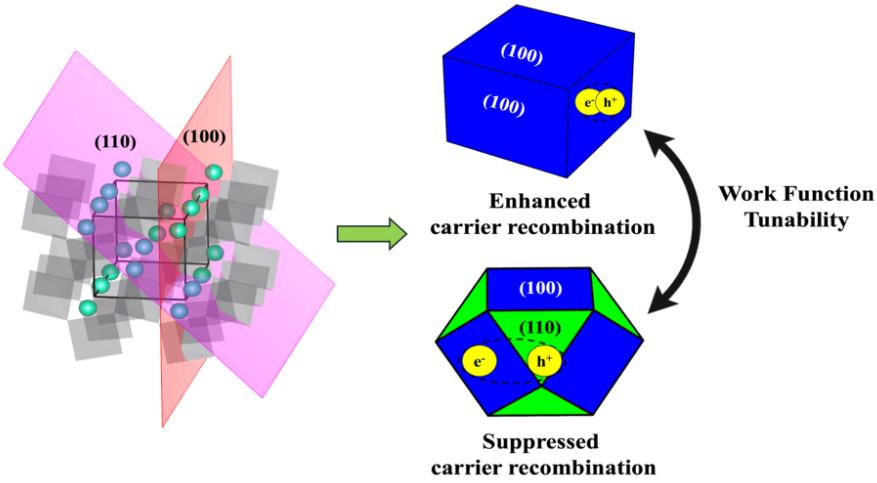


Figure 1. Schematic representation of the bulk crystal structure of $CsPbBr_3$ and the evolution of faceted NCs featuring exposed (100) and (110) facets and the tuning of optoelectronic properties.

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The Pre-organised Enzymatic Electric Field Enables Efficient Carbene Transfer in Artificial Heme-Containing Toroidal Scaffold than Conventional Heme-Myoglobin

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Enzymes are nature's ultimate catalysts that catalyse several complex reactions efficiently but very specifically. Among several enzymes, the heme-containing metalloenzymes such as Cytochrome P450 and Myoglobin are some of the best-known catalysts that catalyse a plethora of reactions, such as C—H activation, sulphoxidation, epoxidation, and many more. A very recent study by Baker et al. designed an artificial heme-containing enzyme that catalyses the carbene transfer very efficiently.[1] However, a mechanistic study and the rationale for why this artificial toroidal scaffolded enzyme is superior to the naturally occurring Myoglobin enzyme were not elucidated. In this study, using sophisticated computational chemistry tools, such as MD simulations, DFT, and hybrid QM/MM calculations, we show that the pre-organised local electric field of the artificial enzyme facilitates efficient carbene transfer. We comprehensively studied the mechanism of the carbene transfer and compared it with that of Myoglobin. The quantification of the pre-organised electric field in the artificial and the Myoglobin indicates an extensive electrostatic field projected along the heme iron-oxo in the Toroidal scaffold compared to the naturally occurring Myoglobin. This work underscores the transformative potential of computational enzyme design in creating biocatalysts with tailored electric fields,[2] presenting a new approach to enhance reaction specificity and efficiency.

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Dynamics of Excited State Proton Transfer in [2,2'-Bipyridyl]-3,3'-diamine

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In this work we reinvestigated the dynamics of excited state proton transfer in [2,2'-bipyridyl]-3,3'-diamine, or $Bp(NH_2)_2$. Femtosecond fluorescence upconversion spectroscopy study by Toele and Glassbeek identified two emission bands followed by photoexcitation, both decaying in about 250 fs and having low fluorescence quantum yield. These bands were identified as the diamine (DA) emission at lower wavelength and diimine (DI) emission at longer wavelength. Ortiz-Sanchez et al. performed computational study on this system and revealed that DI is unlikely to be formed and instead attributed the spectroscopic signals to be associated with the monoamine (MI) and its twisting on a timescale of 250 fs. Chaihan and Kungwan performed surface hopping simulations on the system and found only the MI form upon photoexcitation and the proton transfer timescale is also well matched with the experimental timescale. We have revisited the molecule in this work. We have used surface hopping simulations to study the proton transfer dynamics and decay rate of the experimental fluorescence signals. We found that the molecule exists in two ground state minima of C_2 and C_i symmetries, respectively, while only C_i form exists on the lowest bright state. Dynamics on the S_1 state reveals that only single proton transfer takes place leading to the MI form. Our dynamics suggest that the ~250 fs timescale observed in the experiments may indeed arise from the twisting of the bipyridyl rings over the timescale after SPT, as suggestedin the former computational study.

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Simulating Light-Matter Interactions: From Attochemistry to Nanoplasmonics

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Light-matter interactions are fundamental to diverse areas of research as they find interesting applications in science and technology. On the sub-femtosecond to attosecond timescales, it has gained a lot of attention as it allows the study of ultrafast molecular dynamics with unprecedented time resolution.[1] To this end, I will introduce the concept of quantum coherence to address the question: how long does electronic coherence retain in polyatomic systems in presence of nuclear degrees of freedom?[2]

Research on the interaction of light with the free electrons in metal nanoparticles is also a topic of continuing interest due to their ability to support surface plasmon resonances. Hybrid plasmonic-photonic modes associated with lattices of plasmonic nanoparticles show high quality factors,[3] making them suitable for widespread applications. To this end, I will show how lattice plasmon modes can act as efficient mediators in funneling molecular excitation energy and demonstrate the possibility of achieving long-distance energy transfer.

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Deciphering Tobacco-Induced Regioisomeric DNA Adducts via Artificial Intelligence-Enabled Quantum Sequencing

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Tobacco smoke contains a wide spectrum of genotoxic carcinogens that interact with DNA to generate structurally diverse regioisomeric adducts. These adducts are central to mutagenesis and carcinogenesis, yet their accurate detection remains challenging due to subtle structural variations. Over the past few decades, conventional sequencing techniques such as LC/MS and GC/MS have demonstrated remarkable analytical power; however, their broader applicability is hindered by high operational costs and technical complexity. Advances in biological nanopore-based next-generation sequencing have addressed some of these challenges but remain limited in scope. In this work, we propose an AI-driven graphene nanogap framework that integrates a semi-supervised learning (SSL) model with a quantum transport (QT) approach for site-specific identification of tobacco smoke–induced DNA adducts.[1,2] The complete workflow of our methodology is illustrated in Figure 1.4. Our framework demonstrates high-throughput, rapid, and single-base resolution sequencing, achieving an impressive classification accuracy of 94%, thereby establishing a robust proof-of-concept for precise adduct detection.

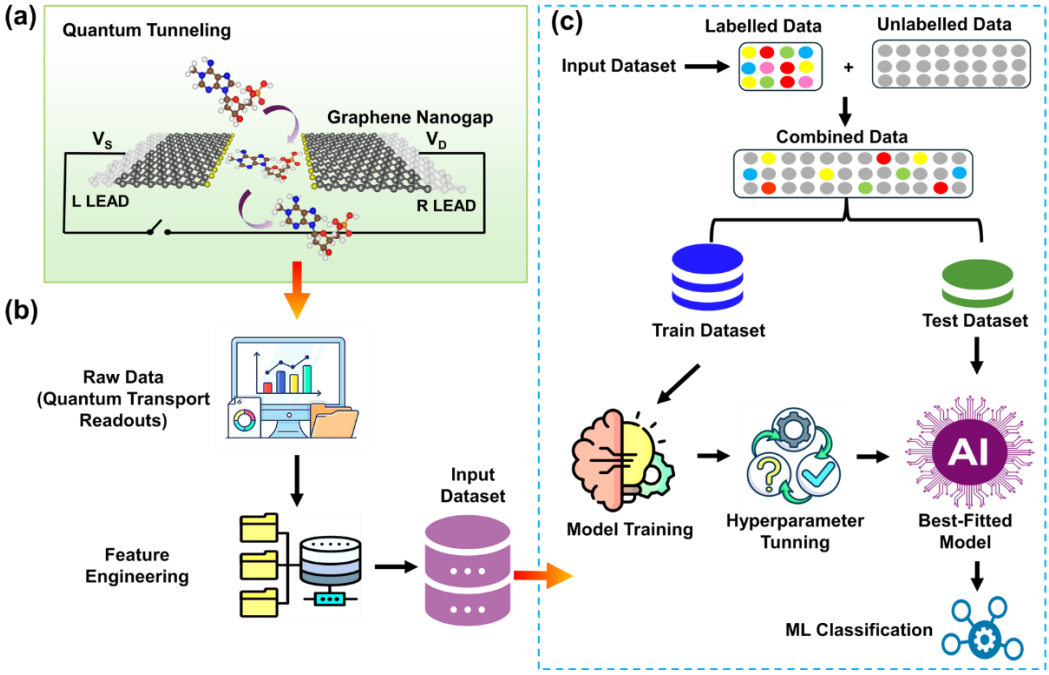


Figure 1 Illustration of the integrated workflow combining (a) quantum tunneling, (b) data acquisition, and (c) SSL for the classification of regioisomeric DNA adducts through a hydrogen-terminated graphene nanogap device.

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Molecular Dynamics Guided Binding Free Energy Analysis of Superior Antitubercular Activity of Imidazo[1,2-a]Pyrimidine-Triazole Hybrids

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Tuberculosis (TB) remains a leading global health challenge, with the emergence of drug-resistant strains limiting the effectiveness of existing therapies such as isoniazid (INH). Our recent synthesis of imidazo[1,2-a]pyrimidine-1,2,3-triazole hybrids identified compound P15 as the most potent antitubercular agent against Mycobacterium tuberculosis H37Rv, with a minimum inhibitory concentration (MIC) of 6.75 μM, outperforming P3 (12.05 μM), P13 (11.95 μM), and the reference drug isoniazid (INH).

Molecular dynamics (MD) simulations revealed that LIG15, one of the novel ligands, exhibited superior binding characteristics compared to INH. It maintained a more stable protein structure, with a radius of gyration (Rg) of approximately 2.12-2.14 nm compared to INH's 2.16-2.18 nm. Root mean square fluctuation (RMSF) analysis showed that LIG15 effectively reduced flexibility in key binding regions. MM-PBSA calculations indicated binding free energies of -149.865 ± 12.591 kJ/mol for P15, significantly stronger than INH's -35.292 ± 9.434 kJ/mol. This confirmed P15's approximately 4.2-fold greater binding affinity over INH.

The results provide a solid basis for P15's exceptional antitubercular activity, with ongoing simulations further clarifying the binding mechanisms for rational optimization of this promising lead compound.The enhanced dynamic stability and superior binding free energy of P15 provide the structural and thermodynamic basis for its exceptional antitubercular activity. Ongoing enhanced sampling simulations are further elucidating the binding mechanisms to guide rational optimization of this promising lead compound for antituberculosis activity.

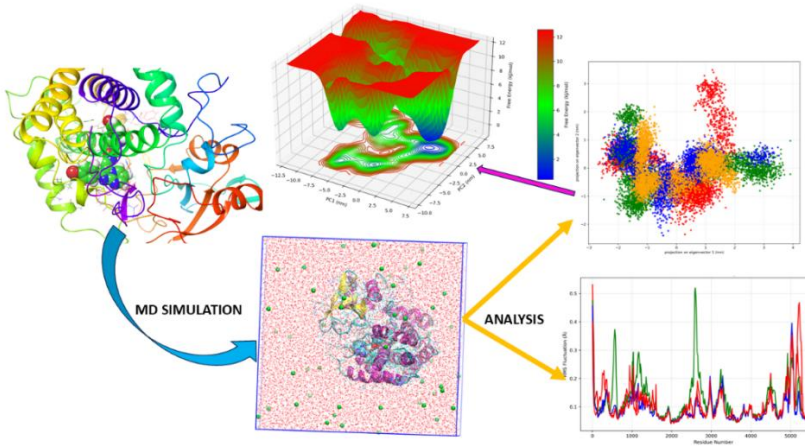


Figure 1. Time Evolution of a 4KTF-Drug Complex from Molecular Dynamics

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Theoretical Chemistry Symposium
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Efficient Hydrogen Storage in Strain Induced Boron Phosphide Biphenylene

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The storage of hydrogen energy is the main obstacle to its widespread use, emphasizing the necessity for efficient storage material [1]. Motivated by the increasing prevalence of inorganic biphenylene substitutes, we investigated strain-induced modulation of hydrogen storage in boron phosphide biphenylene (BPB) via first-principles calculations [2]. Pristine BPB is an inefficient substrate for hydrogen storage since the average adsorption energy of 24 H_2 molecules is –0.17 eV/H_2, which falls below the DOE requirement. Thus, we studied the hydrogen storage capacity of the BPB monolayer under uniaxial (U-BPB) and biaxial strain (B-BPB). Compressive strain enhances bond electronic density, strengthening H_2 adsorption and increasing adsorption energy, whereas tensile strain offers no potential for storage. On the application of 2.25% uniaxial strain along the x and y directions and 1.25% biaxial strain, BPB is able to adsorb 24 H_2 molecules, achieving a storage capacity of 8.8 wt% with corresponding average adsorption energies of –0.22, –0.26, and –0.25 eV/H_2, respectively (Figure 1). AIMD simulations and force constant calculations establish thermal and dynamical stability of the strained BPB monolayers. The work emphasizes strained BPB as a versatile reversible hydrogen storage material.

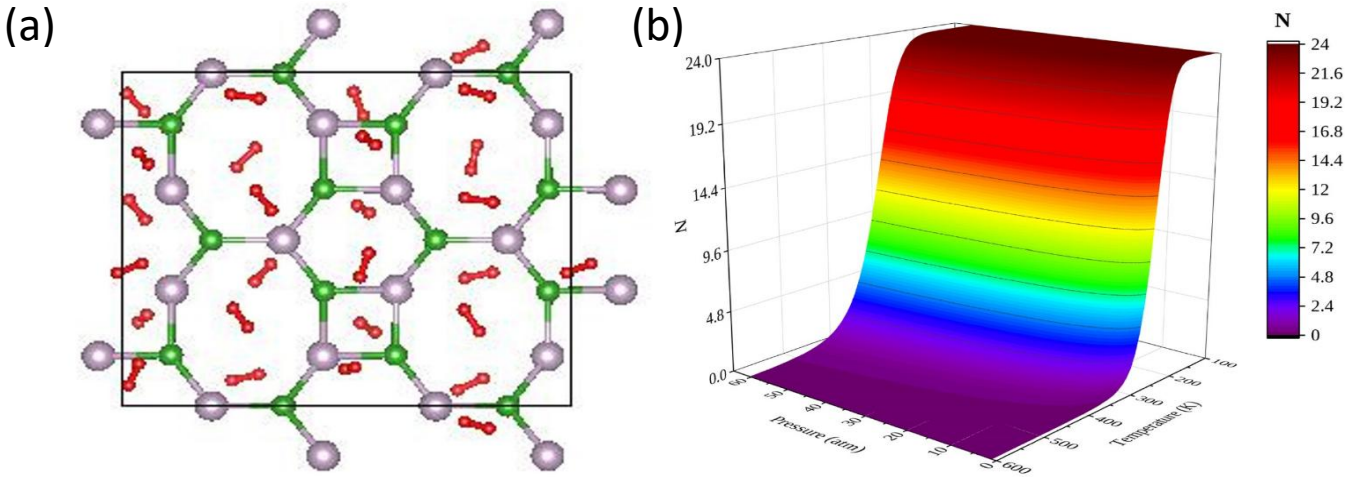


Figure 1. (a) Relaxed structure of 24H_2@1.25%B-BPB system. Atom color representation: B-green, H-red and (b) Hydrogen occupation number as a function of temperature and pressure on 1.25%B-BPB system.

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Reversible Hydrogen Storage in Alanates: A DFT Study

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The reversible storage and utilization of hydrogen has become dominant over the years due to its less impact on the environment regarding climate changes. Number of compounds are identified to have good hydrogen storage capacity, volumetrically and gravimentrically[1]. Aluminium hydrides (Alanates) are one among them. Seven different polymorphs of alane (AlH_3) are identified till date among them α, ά, β and γ alanes are most stable, thermodynamically[2]. Earlier Density Functional Theory (DFT) studies have proved that these plymorphs shows phase transition with increase in pressure[3]. Here, we are investigating the structure, stability, pore size and bond strength in different alanates to see how these factors influence the reversible H_2 storage in them. The molecular hydrogen may affect the bonding strength of Al-H and H-H bonds in these alanes. The role of the interstitial hydrogen molecule in bond strength and, consequently, in hydrogen storage capacity is analyzed through DFT studies.

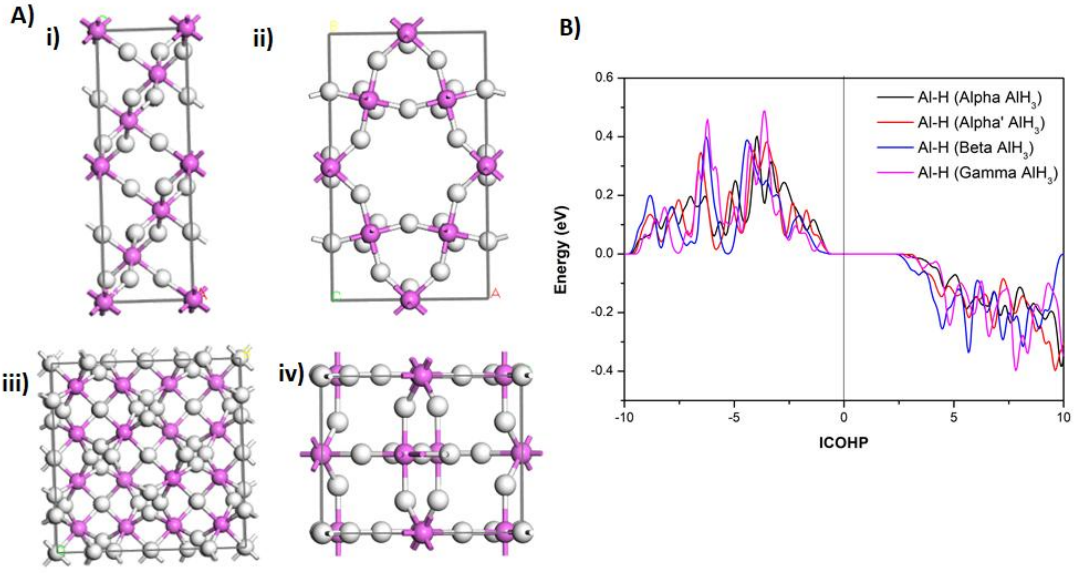


Figure 1 A) Optimized geometries of different polymorphs of alane i) α AlH_3 ii) ά AlH_3 iii) β AlH_3 iv) γ AlH_3. B) ICOHP plots for Al-H bond in different polymorphs od AlH_3

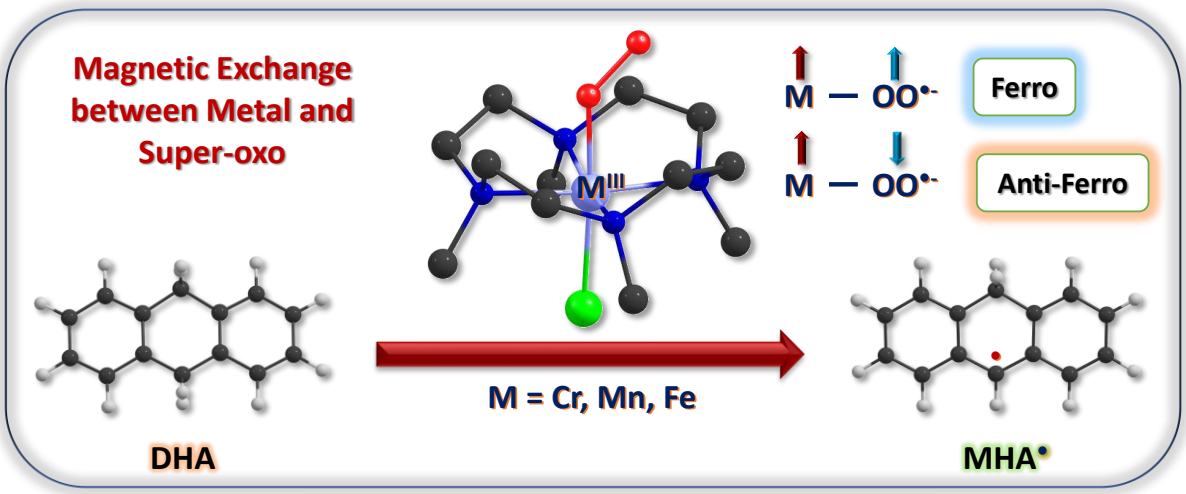
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Understanding Magnetic-Exchange Effects in Metal-Superoxo Species Involved in C–H Bond Activation

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Metal-superoxo species are ubiquitous intermediates in metalloenzymes and bioinorganic chemistry, well-known for their noticeable reactivity and their ability to mediate the activation of inert C–H bonds.[1-4] Despite their biological and catalytic significance, the inherent chemical properties of metal-superoxo complexes remain incompletely characterized and continue to present substantial conceptual challenges.[5] In the present study, we employ state-of-the-art density functional theory (DFT) methods to elucidate the geometric and electronic structures, spin-state energetics, and mechanistic pathways that govern C–H bond activation by high-valent metal-superoxo systems. Particular attention is directed toward outlining the influence of magnetic exchange interactions on the activation barriers associated with C–H bond activation. A comparative assessment of the oxidative capabilities of M–$O_2^{\bullet-}$ species (M = Cr^{3+}, Mn^{3+}, and Fe^{3+}) reveals that Fe^{3+} and Mn^{3+}–superoxo complexes exhibit prominently higher oxidizing power than their Cr^{3+} counterparts, implicating the magnetic exchange parameter as a key determinant of reactivity. Collectively, this work provides new mechanistic insights into the activation of inert C–H bonds by high-valent metal-superoxo species and advances the fundamental understanding of their electronic and magnetic characteristics.



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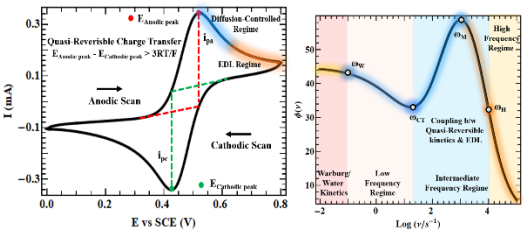
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Admittance of Quasi-Reversible Charge Transfer with Antagonistic EDL on Heterogeneous and Rough Electrode Surface

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A modular theoretical approach is developed to unify ubiquitous electric double layer (EDL) dynamics along with quasireversible charge transfer (QCT) and migration at heterogeneous and rough electrodes. The EIS response include contributions of DC-bias (EDC), standard rate constant (k^0), electroactive concentration, and ohmic resistance on coupled EIS response, extending from quasireversible to reversible limits, are discussed. Theoretical EIS response has three frequency regimes: (i) high frequencies ($\omega > \omega_H$), governed by diffuse-EDL dynamics and solution resistance, (ii) intermediate frequencies ($\omega_H \geq \omega \geq \omega_{CT}$), with DC-bias (wrt to formal potential, $E^{0'}$) in range of RT/F to 3RT/F, governed through coupling between QCT and EDL dynamics, and (iii) low-frequency anomalous Warburg diffusion regime ($\omega < \omega_{CT}$). Electrode heterogeneity causes distributed sluggish charge transfer kinetics of electrolyte/solvent decomposition coupled to EDL reflected through phase suppression. EIS of QCT has a phase minimum governed by E_{DC}, k^0, and electroactive concentration in the intermediate frequency. The dynamic interplay/coupling of EDL and QCT kinetics govern the appearance and disappearance of phase minimum. Finally, theoretical outcomes are validated experimentally using the Fe^{2+} /Fe^{3+} redox couple in $HClO_4$, and this model is also suited for half-cells of devices, viz., SiNW-anode in Li ion half-cells, to emphasize a wider applicability of theory in electrochemical devices

Figure 1 Representation of energy scales using cyclic voltammogram and time dependent illustration of various electrochemical processes for EDL dynamics coupled with QCT.



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Impacting Drug Discovery Programs with Large-Scale De novo Design: AutoDesigner, CoreDesign, and Active Learning FEP+

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The Hit-to-Lead (H2L) and Lead Optimization (LO) stages of small-molecule drug discovery are severely constrained by the Multiparameter Optimization (MPO) problem and the resource-intensive nature of synthesizing and assaying compounds. Traditional computational and medicinal chemistry methods often lead to limited and inefficient exploration of the vast chemical space, contributing significantly to high attrition rates.

To overcome these bottlenecks, we introduce AutoDesigner, a revolutionary de novo molecular design platform. AutoDesigner operates through an Active Learning (AL) feedback loop, tightly integrated with Free Energy Perturbation (FEP+) calculations (AL-FEP+). FEP+ is a rigorous, physics-based method used to calculate the free energy difference (ΔG) between two molecular states. In drug discovery, it is used to calculate the relative binding affinity (ΔΔG) of a modified compound compared to a reference compound. By integrating Free Energy Perturbation (FEP+) engine and 'Active Learning' framework together we can intelligently prioritize compounds—both highly potent and structurally novel. The AL-FEP+ workflow enables the rapid profiling of virtual compounds based on predicted binding affinity and a multi-parameter druggability score. Eventually it minimizes the wet-lab synthesis and assaying of low-value molecules. The result is a transformative acceleration of the Hit-to-Lead and Lead Optimization phases and expanding the accessible chemical diversity for challenging targets. AutoDesigner represents a critical shift from manually driven SAR exploration to truly computer-driven molecular design.

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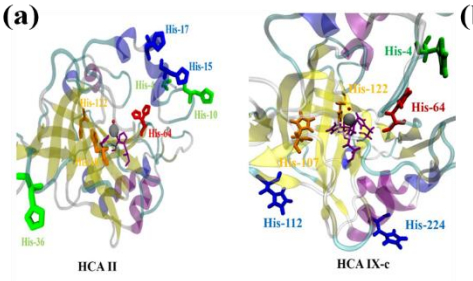
Theoretical Chemistry Symposium
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Conformation-Dependent pK_a of Histidine Side Chains: A Case Study in the Isozymes II and IX of Human Carbonic Anhydrase

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Extensive constant pH replica-exchange molecular dynamics (CpH-REMD) simulation studies on the isozymes II and IX human carbonic anhydrase (HCA) in water have been carried out to compute the pK_a of the side chains of all histidine residues with varying degrees of solvent exposure and relevance in the catalytic function.[1] First, for HCA II, the estimated total pK_a of four non-catalytic His side chains accurately reproduce their experimental values.[2] The observed deviations in the case of three non-catalytic His side chains are attributed to the preferential sampling of one of the possible protonation states dynamically stabilized by $\pi-\pi$ stacking, $cation-\pi$, salt bridge, and hydrogen bonding interactions. Next, the side chain of catalytic His-64 exhibits a higher pK_a in HCA IX than in HCA II. This may be attributed to its preferential outward orientation that persists up to pH 8 thereby stabilizing the protonated state and shifting the pK_a upward. Both isozymes are found to exhibit the emergent concept of conformation-dependent side chain pK_a of catalytically important and non-catalytic His residues. The most important evidence is provided by a quantitative agreement between the estimated side chain pK_a of two different conformations of His-64 side chain in HCA II with the values measured in recent NMR studies.[3]

(a)



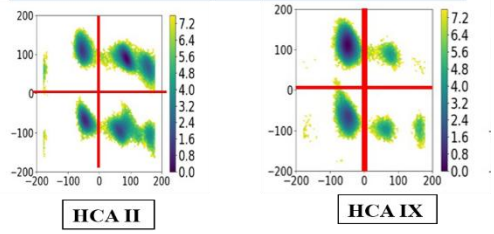
(b)

Comparison with experiment		
Residue	CpH-REMD	NMR
His-4	4.00 ± 0.02	6.20 ± 0.10
His-10	5.45 ± 0.01	5.60 ± 0.10
His-36	6.80 ± 0.01	6.94 ± 0.20
His-15	5.57 ± 0.03	5.60 ± 0.10
His-17	4.09 ± 0.01	5.60 ± 0.01
His-64	6.88 ± 0.03	7.12 ± 0.04
His-107	5.68 ± 0.03	< 3.5
His-122	3.62 ± 0.09	< 3.5

(c)

Comparison between HCA II & IX				
	HCA II		HCA IX-c	
Type	Residue	pK_a	Residue	pK_a
Highly exposed to solvent	His-4	4.00	His-4	6.30
	His-10	5.45		
	His-36	6.80		
Moderately exposed	His-15	5.57	His-112	7.29
	His-17	4.09	His-224	5.76
Low exposed	His-64	6.88	His-64	8.28
Buried	His-107	6.68	His-107	5.86
	His-122	3.62	His-122	5.35

(d) Conformation and charge dépendent free energy surface of catalytic His-64 side chain



(e) Conformation dépendent pK_a of catalytic His-64 side chain

Side chain orientation	State	Conformation dependent pK_a	
		HCA II	HCA IX-c
INWARD	B	6.03 ± 0.14	6.55 ± 0.19
	C	6.18 ± 0.05	6.67 ± 0.21
OUTWARD	A	7.99 ± 0.32	9.85 ± 0.07
	D	7.56 ± 0.32	8.67 ± 0.05

Figure 1 : (a) Position of all histidine residue in both isozymes, (b) pK_a of HCA II and comparison with NMR[2] data, (c) comparison of pK_a between HCA II & IX, (d) Free energy surface of His-64 at pH 7 and (e) Conformation dependent pK_a of His-64 of both isozymes.

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Exploring The Rate Of Fluorescence And Intersystem Crossing In Nitrogen Chalcogenide Co-Doped Graphene Quantum Dots With Vacancy Defect.A DFT Study

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Graphene Quantum Dots (GQDs) are known for low toxicity, strong fluorescence, high surface area and tunable band gaps [1]. The preparation process of GQDs can lead to various defects, including vacancy defects, which can affect the electronic, optical and morphological properties [2]. We have explored the rate of fluorescence (fl) and the rate of intersystem crossing (ISC) in co-doped GQD with a vacancy defect. Here, we investigated the impact of chalcogenide doping, such as O, and heavy atoms like S, and Se, at the vacancy sites of GQD, along with N, on the fluorescence and ISC rate. ISC from the lowest singlet excited state (S1) to triplet manifolds that pave the way to produce triplet states (T*n*). In principle, ISC is a spin-forbidden process. However, it occurs through spin–orbit coupling (SOC), which perturbs the wave functions and yields singlet–triplet mixing. The presence of heavy atoms enhanced SOC, resulting in efficient ISC [3]. For calculating the excited state properties, we employed TDDFT and used ωB97X-D/6-31 + G(d,p) basis set. According to first-order perturbation theory, the degree of singlet–triplet mixing (λ) is related to SOC and ΔST as $\lambda \simeq \langle S1|\mathbf{HSO}|Tn\rangle/|\Delta ST|$. Therefore, in conjunction with low ΔST, the nonvanishing SOC effectively mixes the S1 and T*n* states to allow ISC. We explored the possible deactivation from the S1 states of the GQDs and used the Strickler-Berg relationship to find the k_{isc} [4]. The Marcus rate expression is used to calculate the ISC rate constant [5]. All calculations were performed with the DFT using the Q-Chem 5.4 package. It is observed that the highest ISC rate constant is achieved for GQD with Se dopant, with an SOC of 13.3 cm^{-1}, of 10^{10} sec^{-1}, compared to S dopant, 10^{9} sec^{-1} and O dopant, 10^{7} sec^{-1}. The k_{fl} follows the rate order O > S > Se. Our study examined the photophysical properties of co-doped GQD and optoelectronic properties as we go down the group of chalcogens.

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Machine Learning Boosted Quantum-Profiling of Blood Antigens

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The molecular-level characterization of glycans, a challenging yet highly desirable goal, is crucial for the comprehensive advancement of glycosciences. Despite significant advances in analytical techniques, including NMR and mass spectrometry, structural and configurational complexity hinders the ability to identify carbohydrates, especially high-order saccharides with regioisomeric glycosidic linkages. Herein, we present a computational methodology that utilizes a quantum tunneling method coupled with machine learning (ML) to recognize a wide range of blood antigens simultaneously. Random forest classifier with SHapley Additive exPlanations (SHAP) interpretability performs rapid quantum profiling of all considered molecules with good precision and sensitivity. Our proposed ML-enhanced quantum methodology offers a powerful alternative to conventional techniques, facilitating accurate and high-throughput characterization of carbohydrates by performing 'sugar calling' from their transmission signatures.

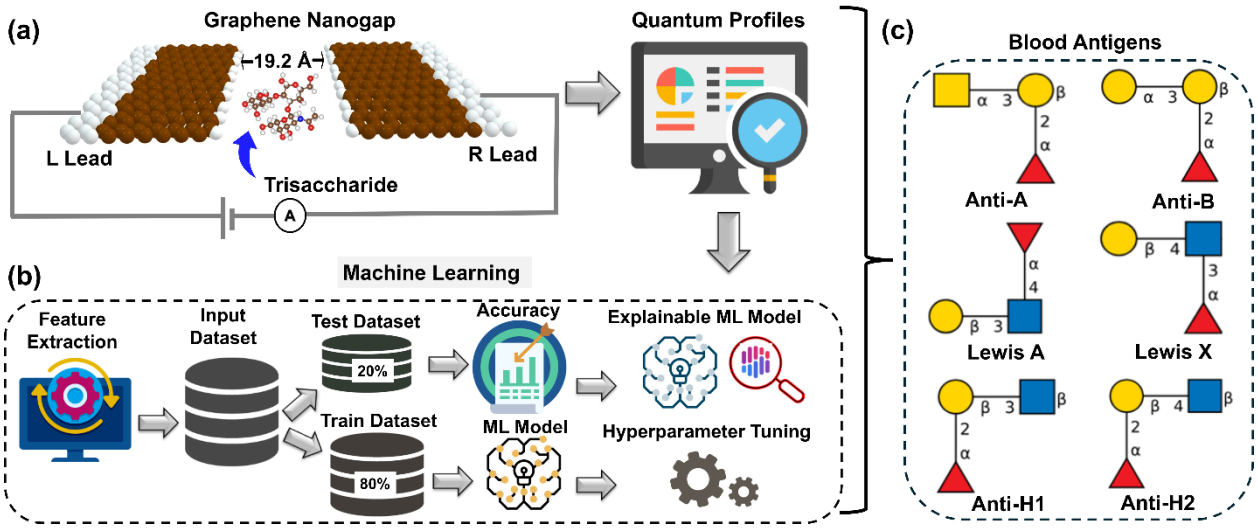


Figure 1 Schematic illustration of quantum profiling of blood antigens coupled with a machine learning (ML) workflow. (a) schematic of graphene nanogap junction in which blood antigens can be trapped in all possible orientations, (b) ML workflow for trisaccharide classification, and (c) symbol nomenclature of targeted blood antigens: Anti-A, Anti-B, Lewis A, Lewis X, Anti-H1, and Anti-H2. As per the symbol nomenclature of glycans, the yellow square represents N-Acetyl-D-Galactosamine (GalNAc), the yellow circle represents Galactose (Gal), the red triangle represents Fucose (Fuc), and the blue square represents N-Acetylglucosamine (GlcNAc).

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MECHANISTIC INSIGHTS INTO AMINOCATECHOL OZONOLYSIS: A THEORETICAL STUDY

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The aromatic amines in the atmosphere, stemming from diverse emission sources, like biogenic and anthropogenic sources, has prompted a theoretical investigation into the gas-phase ozonolysis of substituted catechols[1,2]. Computational methodologies were employed to elucidate the reaction mechanisms, which proceed via (i) 1,3-cycloaddition to form primary ozonides (POZs), subsequent generation of Criegee intermediates (CIs) and (ii) Ozone addition yielding organic hydrotrioxides (ROOOH), alongside other products. Kinetic analyses were carried out to show the temperature-dependent rate behaviours. The Master Equation Solver for Multi-Energy Well Reactions (MESMER) was utilized to calculate rate coefficients for the reactant-to-product transformations, providing insight into the intricate reaction dynamics[3]. This study underscores the significance of electron donating groups in the reactivity of catechols towards ozone.

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Accelerated computational discovery of novel perovskites via first-principles and data-driven approaches

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The perovskite structural framework, characterized by its 1:1:3 ternary composition, holds a pivotal position in materials science due to its remarkable ability to host a vast range of elemental compositions, thereby enabling extensive tunability of physical and chemical properties. This structural versatility underpins its widespread applicability in next-generation technologies, including photovoltaics, superconductivity, magnetism, and catalysis. While perovskites are often regarded as structurally archetypal, their inherent flexibility permits significant deviations from the ideal cubic symmetry. Subtle octahedral tilts, distortions, and compositional substitutions introduce a rich and complex potential energy landscape characterized by multiple polymorphic forms.[1,2] These intricacies complicate the establishment of clear structure–property correlations and render the accurate prediction of stable and metastable phases particularly challenging. In this symposium, we address these challenges by a comprehensive combinatorial framework that integrates theoretical insights, first-principles calculations, and data-driven methodologies.[3,4] We illustrate the prediction of both stable and metastable structures for novel perovskite oxides and chalcogenides, focusing on applications in sustainable energy and quantum materials.[5,6] Our systematic workflow encompasses the prediction of candidate structures, followed by harmonic and quasi-harmonic phonon modelling for rigorous stability assessments under varying pressure-temperature (P-T) conditions.[7,8] Furthermore, based on quasiparticle approximations, we explore the potential optoelectronic properties of the most synthesizable candidates, highlighting their applicability in advanced functional devices.

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Learning Condensed Graph via Differentiable Atom Mapping for Reaction Yield Prediction

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Predicting the yield of a chemical reaction is a fundamental challenge in chemistry. A key determinant of yield is the transition state, a transient high-energy structure. Existing deep learning models often overlook this critical aspect as real-world datasets typically lack any transition state(TS) information. To address this, we introduce YieldNet, a neural network that first approximates atom mapping using a differentiable node alignment module2, allowing it to estimate a continuous condensed graph(CGR)1 of the reaction as a surrogate transition state. This surrogate graph is then processed by input-differentiable graph neural networks and a transformer-based reaction path encoder to predict yields across multi-step reactions. Crucially, the model is trained solely under the distant supervision of reaction yield values, without requiring ground-truth atom mappings or transition states. This enables end-to-end learning of chemically meaningful inductive bias from data alone. This work bridges a key gap between physical chemistry and machine learning, offering a practical tool for chemists to screen and optimize reactions more effectively. YieldNet could accelerate discovery in fields ranging from pharmaceuticals to materials science by reducing the need for costly lab experimentation.

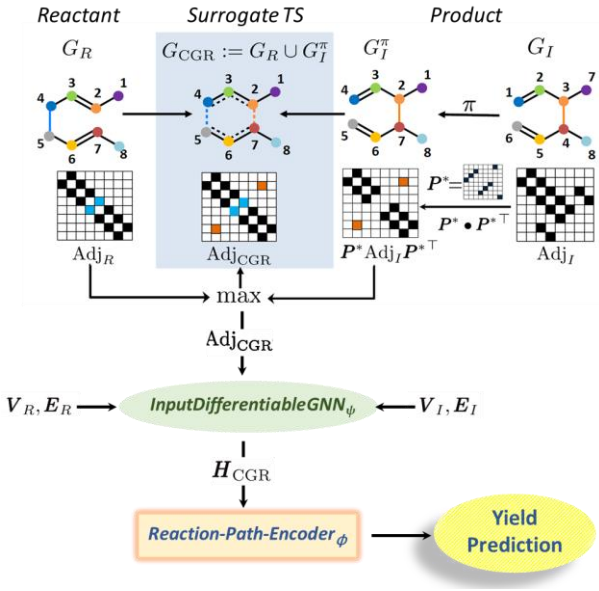


Figure 1 Illustration of YIELDNET. For each reaction step, we feed the node embeddings and edge embeddings into a fully differentiable node alignment network to obtain an alignment matrix P which gives a continuous approximation of the adjacency matrix of CGR, $\mathrm{Adj}_{\mathrm{CGR}}$ and feed this approximate $\mathrm{Adj}_{\mathrm{CGR}}$ with the node and features into a new GNN to obtain $\mathrm{H}_{\mathrm{CGR}}$, the node embedddings of CGR. Finally, a reaction path encoder use $\{\mathrm{H}_{\mathrm{CGR}}\}$ to predict the yield.

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Computational Investigation of NO Adsorption and Underlying Mechanism in Cobalt-Based Metal-Organic Frameworks

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Understanding how open metal sites in metal–organic frameworks (MOFs) mediate small-molecule binding and reactivity is key to advancing selective gas storage and activation. Here, periodic density functional theory (DFT) calculations reveal distinct mechanisms of NO uptake in the isostructural frameworks Co_2Cl_2(bbta) and $Co_2(OH)_2$(bbta). In Co_2Cl_2(bbta), sequential NO adsorption is strongly exothermic for the first molecule but significantly weakened for the second, evidencing negative cooperativity driven by spin-state modulation. In contrast, $Co_2(OH)_2$(bbta) undergoes NO disproportionation upon adsorption, producing N_2O and bound NO_2^- via redox communication across μ_2–OH bridges. Extension across the M_2Cl_2(bbta) series (M = Mn, Fe, Co, Ni, Cu) is done to further understand the role of the metal centre. These results establish that spin-state transitions and intermetallic coupling dictate whether NO binding in MOFs proceeds via reversible adsorption or chemical transformation, offering molecular-level design principles for frameworks that integrate gas storage, delivery, and activation within a single platform.

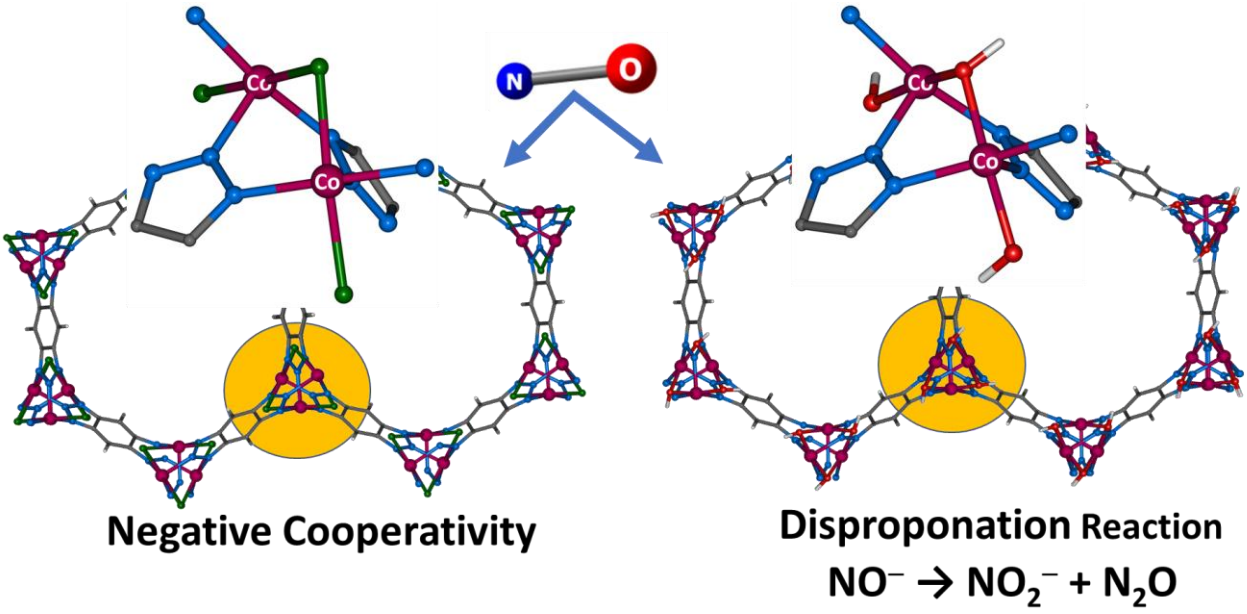


Figure 1 Ligand-dependent NO binding pathways in Co-based MOFs

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Machine Learning Applications for Discovering and Optimizing Singlet Fission Materials in Dye Sensitized Solar Cells

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The Shockley–Queisser limit sets a maximum efficiency for single-junction solar cells. Singlet fission (SF), where one singlet exciton splits into two triplet excitons, offers a way to surpass this limit. For efficient SF, molecules should satisfy the condition $E(S_1) \geq 2E(T_1)$ and $E(T_2) \geq 2E(T_1)$. However, only a few molecules are known to satisfy these criteria, limiting the design of practical materials. In this work, we use generative deep learning with recurrent neural networks (RNNs) to design new SF molecules for dye-sensitized solar cells. A dataset of 262 known SF molecules is expanded via the RECAP algorithm, generating ~400,000 new SMILES strings. A character-level Long Short-Term Memory (LSTM) model is pre-trained on the augmented dataset and fine-tuned on the SF set to capture specific molecular features. Generated molecules were validated using RDKit and duplicates were removed to create a refined library of potential candidates. This framework illustrates the role of machine learning in efficiently identifying promising SF chromophores for future solar technologies.

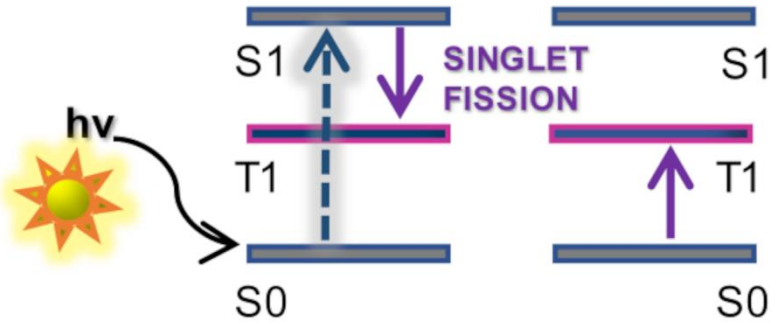


Figure 1: Illustration of the Singlet Fission Process

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Ziegler-Natta Catalyst Systems: "Emergent" Unidirectional Molecular Machines

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Unidirectional biomolecular machines are at the heart of many biological processes, and many machines mimicking such behavior have now been synthesized in the laboratory. What the current work showcases is a new class of unidirectional molecular machines that are neither biological nor consciously designed but are, instead, the outcome of "emergent" behavior in chemical systems. This is shown to be the case in Ziegler-Natta (Z-N) heterogeneous olefin polymerization systems. Calculations with DFT, as well as stochastic simulations, show that the oxygen containing Lewis basic molecule, the "internal donor", successfully and repeatedly finds the active titanium-based catalyst on the $MgCl_2$ surface, due to an "energy ratchet"[1] unidirectional molecular machine being created during the catalysis. Since the presence of the donor at the catalyst centre is a prerequisite for improved stereoselectivity, the formation of "emergent" molecular machines is crucial in Z-N catalyst systems.

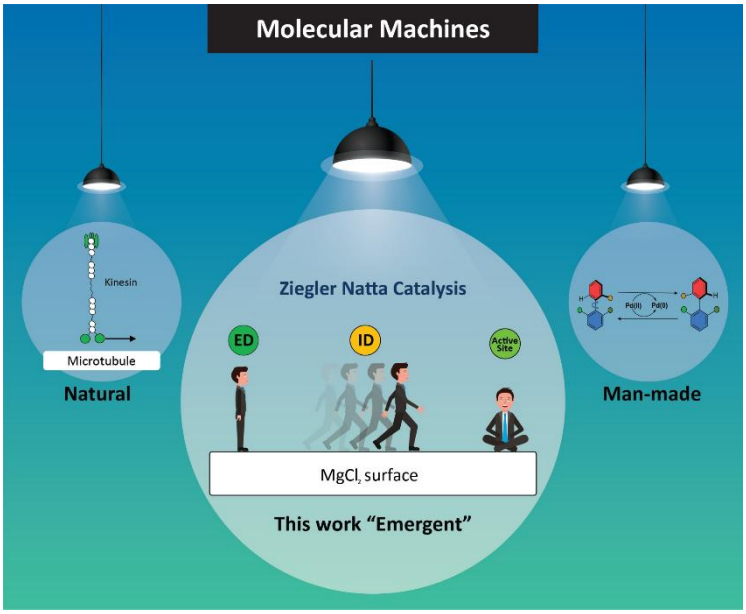


Figure 1: Schematic representation of an internal donor (ID) "walking" on the $MgCl_2$ surface away from an external donor (ED) and towards the active titanium catalyst, showcasing a new class of "emergent" molecular machines.

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Evaluating the preferential adsorption of N_2 from a binary mixture of N_2/O_2 on extra-framework cations of zeolites: a computational and experimental study

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Separation of N_2 from a N_2/O_2 gas mixture is critical for various industrial/medical applications. Temperature/pressure swing adsorption is the top-notch industrial technology used for this separation, where zeolites are the materials used for adsorption. Zeolite X/Y with Li^+ as an extra-framework cation is the best-known sorbent for N_2 gas molecules. However, the present net-zero emission scenario has made lithium a critical element, making it imperative to implement its alternative in various other technologies. In this context, the present work is a computational evaluation to identify a cation that can replace Li^+ for preferential adsorption of N_2 over O_2. The DFT study, based on parameters such as selective adsorption energies of N_2 over O_2 and IR stretching frequencies of the adsorbed N_2 and O_2 molecules, identifies Mg^{2+}, Ca^{2+}, Sr^{2+}, Co^{2+} and Zn^{2+} as potential cations. These cations have preferential adsorption for N_2 over O_2 by 10 kJ mol^{-1} or more. However, BOMD simulations reveal that only Mg^{2+}, Ca^{2+}, Co^{2+} and Zn^{2+} keep the N_2 molecule bound at 300 K, and the O_2 molecule gets desorbed from these frameworks. The desorption temperature of N_2 on Ca^{2+} and Zn^{2+} is 350 K, and on Mg^{2+} is 400 K. These observations are corroborated by electronic charges on cations and molecular orbitals. Significantly, Ca^{2+} is identified to adsorb up to 2 N_2 molecules, making it an ideal candidate for N_2/O_2 separation in place of Li^+. To validate this, we have carried out an experimental study that showed a good N_2 adsorption capacity of 2.1 mmol g^{-1} for Ca^{2+}.

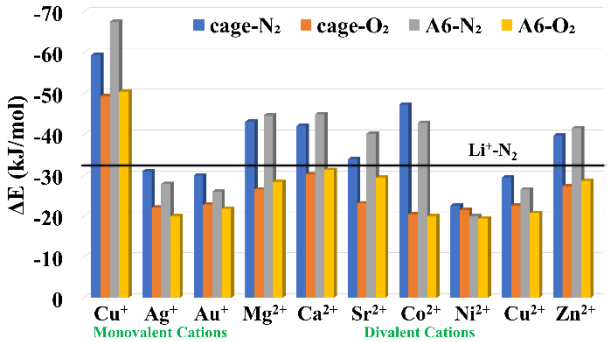


Figure 1 Adsorption energy (in kJ/mol) of the N_2 and O_2 molecules on various cation exchanged sodalite cage and A6 cluster models. The black line passing through the graph is the adsorption energy value of the N2 molecule adsorbed on the Li^+ ion.

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Theoretical Chemistry Symposium
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Mechanistic Insight into Photocatalytic Dry Reforming of Methane on Ni-anchored g-C_3N_4 catalysts: A DFT Study

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Dry reforming of methane (DRM) is a sustainable catalytic route that simultaneously consumes two major greenhouse gases, CH_4 and CO_2, while producing syngas (CO + H_2), a valuable feedstock for fuels and chemicals.[1] Despite its promise, DRM catalysts often suffer from high enegy barriers, poor stability, catalyst sintering, and carbon deposition. To address these challenges, we employed dispersion-corrected density functional theory (DFT-D3)[2] to investigate the catalytic behavior of atomically dispersed and small Ni clusters of varying nuclearity supported on graphitic carbon nitride (g-C_3N_4). Adsorption characteristics, reaction energies, charge density difference (CDD), and charge transfer analysis were systematically analyzed to establish the size-dependent activity and the stability trends. The unique electronic and photocatalytic properties of g-C_3N_4 catalyst, which can harvest visible light to generate electron–hole pairs and promote the dissociation of CO_2 and CH_4, further enhance its potential as a support material for DRM.[3] Based on the calculated Gibbs free energies, we studied all possible intermediates for various elementary reactions of DRM. Furthermore, we predominantly examined the influence of size and the configuration of cluster and the single atom on challenging photocatalytic activation of the inert C-H and C=O bonds of CH_4 and CO_2.[4] The outcomes of this study provide a theoretical basis for the rational design of catalysts for DRM with improved activity, stability, and resistance to carbon deposition, while also highlighting their promise in photocatalytic DRM applications.

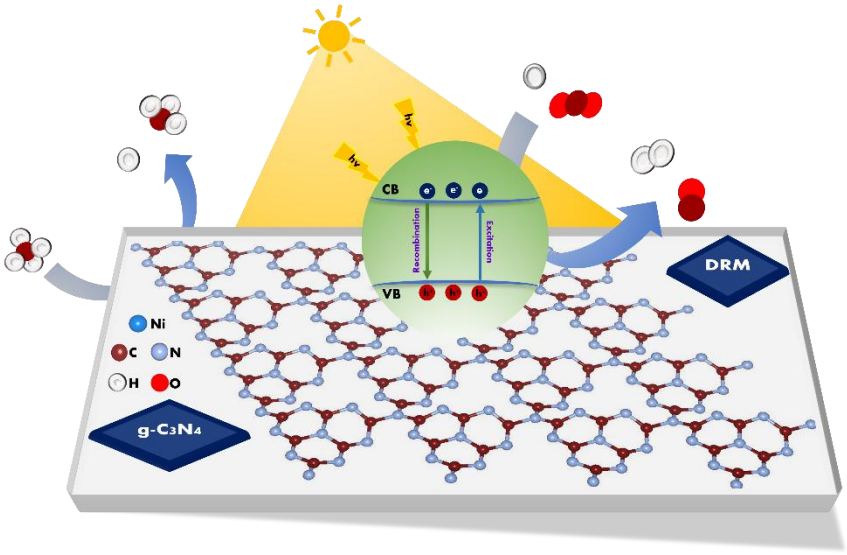


Figure 1. Graphical representation of photocatalytic dry reforming of methane on Ni atom/ cluster modified g-C_3N_4.

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Theoretical Chemistry Symposium
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Tuning CO_2 Activation via Choline–Amino Acid Ionic Liquids on Au(111): A First-Principles Study

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The efficient transformation of CO_2 into value-added chemicals is a key strategy in the pursuit of carbon-neutral technologies. Realizing this goal requires the development of sustainable and environmentally benign catalytic systems, especially within the fields of green chemistry and materials science.[1] The biocompatible nature of ionic liquids has gained attention because of their tunable physicochemical properties, environmental compatibility, excellent recyclability, and eco-friendly character, making them suitable for CO_2 conversion into value-added products utilizing renewable energy sources. Reaction intermediates such as *COOH and *HCOO were examined, and the energy landscape was mapped using nudged elastic band (NEB) analysis.[2] The results reveal that the interfacial environment significantly influences both the activation barriers and the stability of the transition states. This study provides a molecular-level understanding of amino acid-based ionic liquids (AA-ILs) in CO_2 conversion using first-principles approaches.

(a) (b)

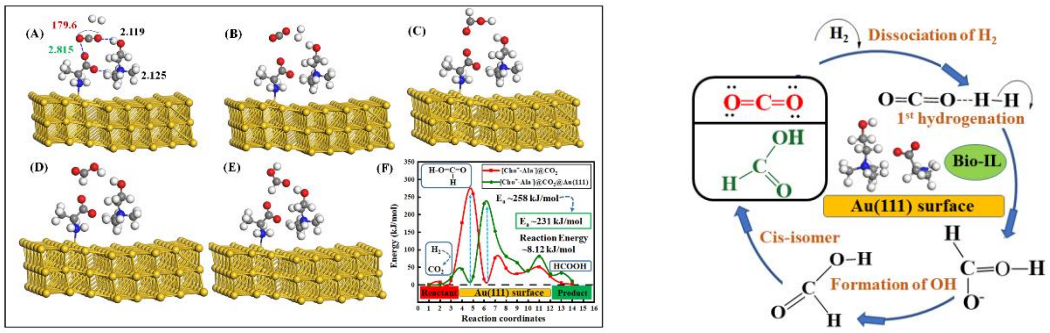


Fig. 1 (a) Simulation of the reaction mechanism between H_2 and CO_2 to form HCOOH at the Bio-IL@Au (b) Schematic diagram of the catalytic reaction mechanism.

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Deciphering the Mechanism Behind the Ortoleva-King Type Reaction:A DFT Perspective

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Imidazo [1,2-α] Pyridines represent a pivotal class of compounds in pharmaceutical research, recognized for their extensive range of biological activities, including potent anti-tumor and anti-cancer properties. This study provides a comprehensive quantum chemical investigation into the mechanism of iron/iodine-catalyzed Ortoleva-King protocol, which offers a highly efficient route for the synthesis of these valuable fused heterocycles. Utilizing a cost-effective and readily available catalytic system comprising FeCl3·6H2O and molecular iodine, this methodology enables the synthesis of various Imidazo[1,2-α] Pyridine derivatives with impressive yields. The reaction, notable for being ligand-free employs chlorobenzene as the solvent. All calculations were performed using the unrestricted M06X functional with the def2-SVP basis set providing a rigorous theoretical framework. The catalytic species were investigated and the energy pathway was calculated. The proposed reaction mechanism involves a four-step pathway involving: Activation of the methyl group via molecular iodine, followed by addition of nucleophilic aminopyridine, water mediated cyclization to form the imidazo moiety, and concluding with dehydration to yield the final imidazo[1,2-α] pyridine product. The water mediated cyclization in a non-aqueous medium presented in this work is mechanistically intriguing. This work makes a significant contribution to the field by presenting an accessible and scalable method for synthesizing biologically important Imidazo[1,2-α] pyridines,with promising implications for drug discovery and development. The work elucidates the importance of a theoretical and experimental approach for designing efficient reaction mechanisms in the field of organic synthesis reactions.

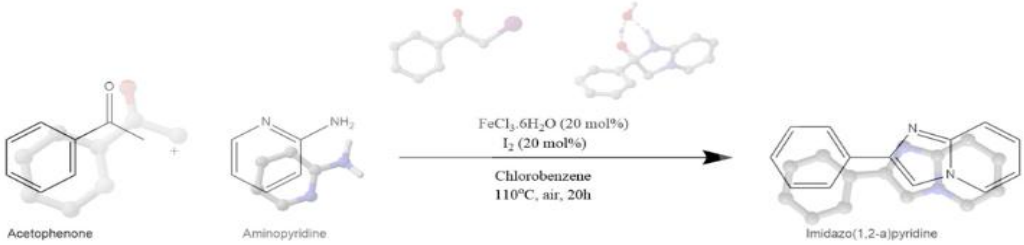


Figure 1 Mechanism of Ortoleva-King reaction

References:

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Theoretical Chemistry Symposium
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Mechanistic Insights into the Molecular Mechanism of Cu-Catalysed Suzuki Miyaura Cross-Coupling Reaction

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The ligand-assisted Cu(I)-catalyzed Suzuki–Miyaura cross-coupling (SMC) reaction was examined to elucidate the mechanistic role of ligand coordination in establishing copper as a sustainable alternative to palladium catalysis. Using Density Functional Theory (DFT) calculations, the C(sp)–C(sp^2) coupling between phenylboronic acid and 1-bromo-2-phenylacetylene in ethanol was investigated with a CuI/8-hydroxyquinoline catalytic system and Na_3PO_4 as the base. The active species was identified as an 8-hydroxyquinoline-ligated Cu(I) complex, stabilized through strong coordination interactions. The catalytic cycle was determined to proceed via an initial transmetalation step, followed by a concerted oxidative addition–reductive elimination sequence, affording the biaryl product in a single step. The computed activation barrier of 18.3 kcal mol^{-1} was found to be consistent with experimental conditions. Importantly, ligand coordination was shown to stabilize both intermediates and transition states, thereby lowering the overall energy profile of the reaction. These findings provide deeper insight into the role of ligand assistance in Cu-catalyzed cross-coupling and underscore its potential as a cost-effective and versatile method for C–C bond formation in the synthesis of pharmaceuticals, agrochemicals, and natural products.

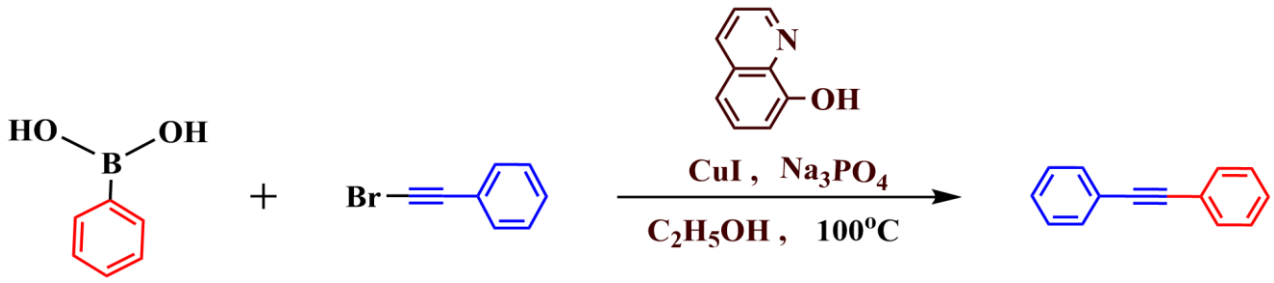


Figure 1 : Model Reaction Mechanism for Cu-Catalyzed Suzuki-Miyaura Coupling

References:

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From Gas to Solution Phase: A Computational Investigation of Halide Recognition via Chalcogen Bonding

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This study rigorously investigates the role of highly directional chalcogen bonding as a master key interaction for anion recognition[1]. This is achieved by designing derivatives of (benzo)chalcogenadiazoles (X = S, Se and Te, Figure 1) for selective binding of halides (F^-, Cl^-, Br^-, and I^-). Quantum chemical tools, including molecular electrostatic potential (MEP) surface qualitatively provide the electronic landscape, demonstrating how the distance and electronic influence of the ring substituents modulate the σ-hole of the chalcogen atom, thereby governing the initial interaction with the anionic species. A detailed quantitative description of binding strength and nature is achieved through symmetry-adapted perturbation theory (SAPT), natural bond orbital (NBO), and quantum theory of atoms in molecules (QTAIM). All these methodologies converge to support a coherent interpretation. On keeping the bis(trifluoromethyl)telluradiazole scaffold constant, we observe a decrease in binding affinity as the halide radius increases down the group, suggesting a diminished selectivity toward heavier halides in terms of energy. Conversely, for the chalcogen donors, binding affinity towards an anion consistently increases with atomic size, following the order S < Se < Te. The nature of the binding is identified to be partially covalent, with the notable exception in the selective recognition of bromide and iodide by benzothiadiazole, which is characterized as noncovalent. Furthermore, the interplay of aprotic and protic solvents was evaluated using the Solvation model based on density (SMD), which depicted the hierarchy of interaction energy, as $E_{gas} > E_{THF} > E_{water}$. These comprehensive computational insights will aid rational design of novel chalcogenadiazole-based receptors and sensors, facilitating advancement in anion recognition for applications in environmental monitoring, sensing, and biomedical remediation[2].

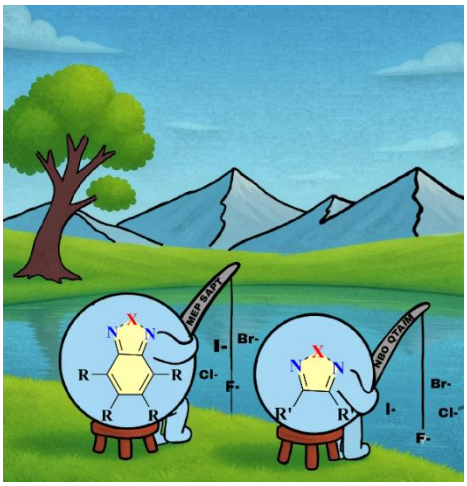


Figure 1: Recognition of anions by chalcogen donors

References:

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Theoretical Chemistry Symposium
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Conformational Preferences of Phenylalanine Heptapeptide: A Molecular Dynamics and Metadynamics Investigation

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Aromatic amino acid–rich peptides display intricate folding dynamics governed by the interplay of π–π interactions, hydrogen bonding, and steric effects. In this study, we examined the conformational landscape of a Phenylalanine heptapeptide, $(Phe)_7$, using classical molecular dynamics (MD) and well-tempered metadynamics (WT-metaD) simulations, with OPLS-AA force field in explicit SPC/E water. Classical MD simulations of 2 μs were carried out from both α-helical and random coil starting geometries to explore their structural evolution. Irrespective of the initial conformation, both trajectories became trapped in compact β-hairpin-like minima, indicating an intrinsic tendency of Phenylalanine-rich sequences to populate turn-containing conformations. To overcome sampling limitations, the enhanced sampling technique WT-metaD was employed using radius of gyration (Rg) and backbone RMSD as collective variables. The free energy surface obtained from the random coil revealed two distinct minima corresponding to β-hairpin and extended coil conformations, whereas the helix-initiated heptapeptide exhibited a more rugged landscape characterized by one global minima and three metastable basins—helical, β-hairpin, and two random coil states, respectively. These findings reveal a complex, multi-minima energy surface dominated by β-hairpin configurations, underscoring the utility of enhanced sampling in capturing the rich conformational diversity of short aromatic peptides and providing atomistic insights into their folding preferences.

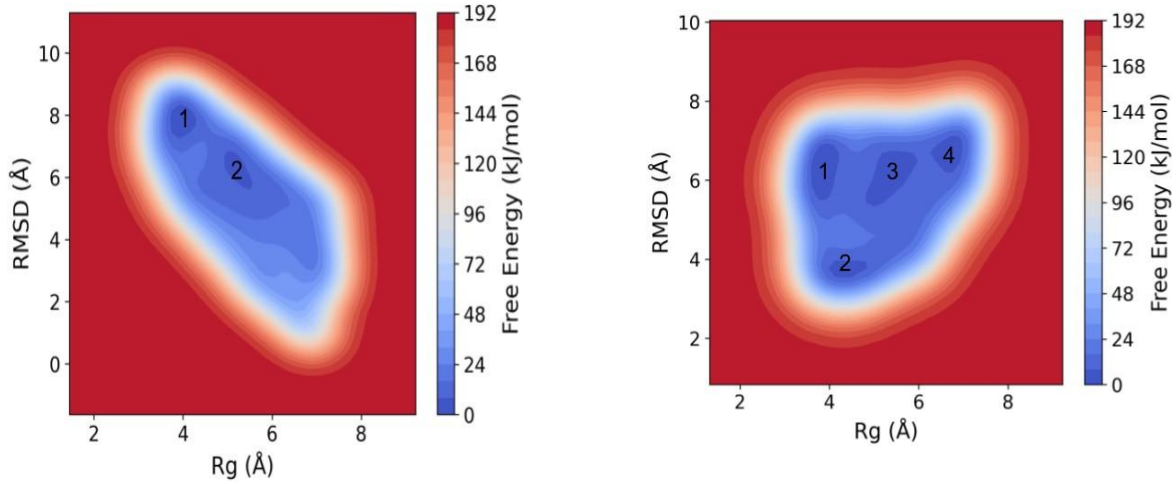


Figure 1. WT-metadynamics free energy surfaces of $(Phe)_7$. Left Randomcoil start (1.β-hairpin, 2.Extended). Right Helical start (1.β-hairpin, 2.Helical, 3 & 4. Extended)

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Mechanistic Insight of Ligand Binding Kinetics with G4-DNA: Insights from FCS and Computer Simulation

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The investigation on ligand interactions with biomolecules in general, focuses on structural and thermodynamical aspects. However, for biomedical and pharmaceutical understanding, the kinetic pathways of ligand/biomolecule interactions has been revealed to be as important as thermodynamics of binding of ligands to its target site, primarily for determining the efficacy of a ligand (or drug).[1–4] For this paramount importance of kinetic aspects of the ligand biomolecule interactions, here we explore the thermodynamic and kinetic pathways of the interaction of a small-molecular benzo[a]phenoxazine and Rhodamine (Rh6G) ligands with parallel G-Quadruplex (G4-DNA) using fluorescence correlation spectroscopy (FCS), well-tempered Metadynamics (WT-MetaDy), and On-the-fly Probability Enhanced Sampling (OPES) simulation methods. The key kinetic parameters, including the association rate constant (k_{on}), dissociation rate constant (k_{off}), are derived experimentally. The findings indicate that the dissociation rate constant, rather than the association rate, remains the primary rate-limiting factor in the binding process. The simulations offer critical molecular level understanding into the thermodynamics as well as the kinetics of ligand interaction, with a particular focus on characterizing the associated free-energy landscape of the ligand/G4-DNA interactions and calculating unbinding rate, which very closely matched with the dissociation rate measured experimentally by FCS. The insights gained here are valuable for drug development and can help in designing ligands with improved specificity toward G4 recognition.

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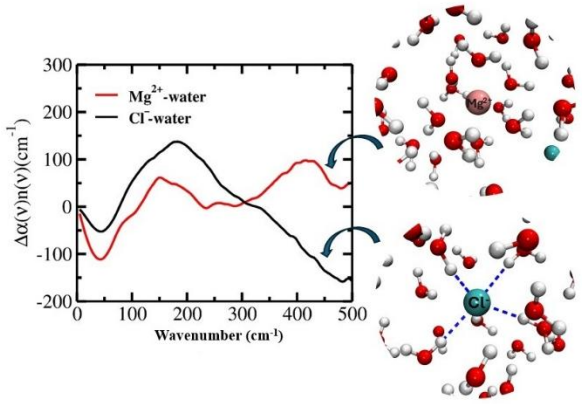
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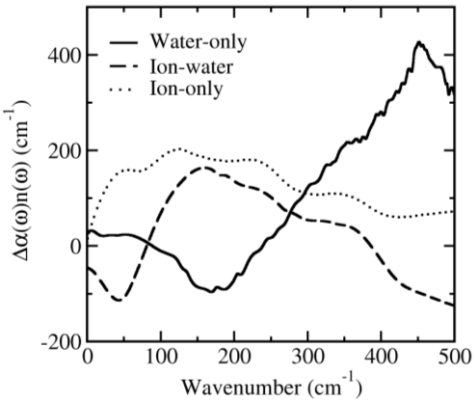
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Terahertz Spectroscopy of Aqueous $MgCl_2$ and $CaCl_2$ Solutions Using Polarizable Forcefields : Intra- and Inter-species Contributions Involving Permanent and Induced Dipoles and Ion Current

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We have investigated the terahertz (THz) [1] and dielectric spectra of aqueous $MgCl_2$ and $CaCl_2$ solutions through molecular dynamics simulations using explicit polarizable force fields for both water and ions. Calculations were performed for three concentrations of each salt at room temperature. The difference absorption spectra were obtained by subtracting the pure water contribution from the total spectra of the solutions. These spectra were further dissected into ion-ion, water-water, and ion-water components,[2] with resolution into self- and cross-correlations. The ion-ion contributions were separated into cation-cation, anion-anion, and cation-anion correlations, while the ion-water parts were divided into cation-water and anion-water interactions. The ion-water contributions were further decomposed into permanent dipole-permanent dipole, permanent dipole-induced dipole, and induced dipole-induced dipole correlations, providing detailed insight into the interactions responsible for the THz response.[3,4] The analyses show that low-frequency modes are mainly dominated by cation-water interactions, with additional contributions from chloride-water hydrogen bond stretch motions. The hydrogen bond stretch motion of water is suppressed by the presence of ions, while additional contribution comes from chloride ion-water hydrogen bonding.[5] These results provide molecular-level insights into ion-ion and ion-water correlations and demonstrate how divalent salts strongly influence the low-frequency vibrational features of water.





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From Discovery to Dynamics: Unlocking Main-Group Reactivity with Aromaticity

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Aromaticity is not only a static feature—it dynamically influences stability, reactivity, and selectivity in main-group chemistry. Our work explores this dual role in two directions. First, using the ab initio nanoreactor (AINR), we uncovered previously unknown cyclic Si–Al rings, including a four-membered 2π-aromatic species capable of activating small molecules such as ammonia. [1] Second, we addressed a fundamental question: how does aromaticity govern the reactivity of N-heterocyclic carbenes (NHCs) along a reaction pathway? By combining electronic, magnetic, and energetic descriptors of aromaticity with activation strain model (ASM) and energy decomposition analysis (EDA), we demonstrate a general principle—preservation of aromatic character lowers activation barriers, while its loss imposes a significant energetic penalty. [2] Together, these findings establish aromaticity as a powerful and tunable lever for molecular design and the development of selective transformations.

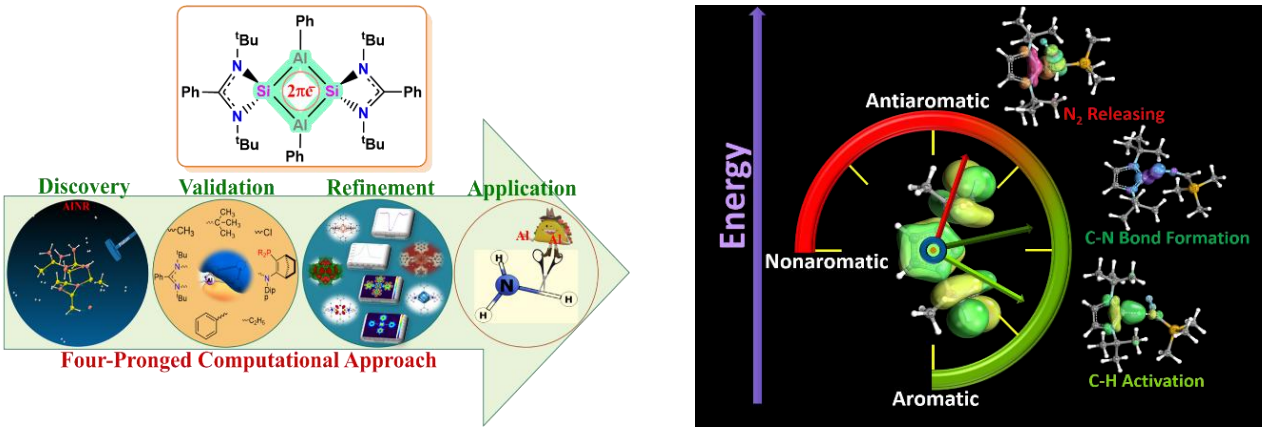


Figure 1 Discovery of a novel cyclic 2π-aromatic Si–Al rings and reactivity of 5-I^{t}Bu with diazo compounds.

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ΔSCF for Excited States Using Parametric Equations of Motion

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The ΔSCF approach is an efficient method for studying excited states in quantum chemistry. This technique involves promoting an electron from an occupied orbital to a chosen virtual orbital; after that, the system is allowed to relax. By obtaining the SCF energy for this excited state configuration and comparing it to the ground state energy, one can calculate the excitation energy and other related properties. However, a significant challenge arises because the relaxation of the non-aufbau system through standard SCF procedures often leads to convergence at the minimum (ground state) instead of the saddle point (excited state). This phenomenon is known as variational collapse.

To address this issue, the Parametric equations of motion (PEM), along with nuclear charge stabilization, are utilized to compute excited state energies. The initial calculation incorporates an additional nuclear charge, which helps ensure that several virtual orbitals of interest (specifically, the LUMO and LUMO+1) are bound. The occupation numbers of the orbitals are then adjusted to generate the desired excited state configuration. Then, PEM calculations are carried out until the additional nuclear charge is gradually reduced to zero, which ultimately yields an SCF solution for the excited state. The key to obtaining a meaningful SCF solution is to maintain fixed occupation numbers for the orbitals involved. By comparing this excited state result with the ground state energies, excitation energies for various systems can be calculated.

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Unravelling Atmospheric Reaction Mechanisms at Seawater: Insights from Ab-Initio Molecular Dynamics Study

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Atmospheric chemistry is significantly influenced by the processes occurring at the seawater. Among these, reactions between halide anions (X^-) present in the water with incoming gas-phase molecules such as hypohalous acid are of major atmospheric interest due to their role in tropospheric oxidation cycle. However, inherent complexity and multi-step nature of these reactions left their mechanisms largely unexplored. Here, we focus on the reactions between hypochlorous acid (HOCl) with anions at seawater in both interfacial and bulk aqueous environmentsusing Ab-Initio Molecular Dynamics (AIMD) simulations. The main findings are:

1) We unravel the detailed atomistic mechanism of halogen exchange reaction, $HOCl+I^- \rightarrow HOI+Cl^-$, which proceeds via a Grotthuss-like hydroxide transport involving multiple water molecules at neutral pH-a stark contrast to the gas-phase mechanism[1].

2) Whereas in acidic pH condition we observe dihalogen formation[2].

3) Intriguingly, we demonstrate the halogen bonded complexes of $[(HOCl)...(X^-)]_{aq}$ act as the reaction precursors while the hydrogen bonded complexes remain unreactive. Our studies suggest that AIMD is a powerful tool to investigate these interfacial charge transfer reactions.

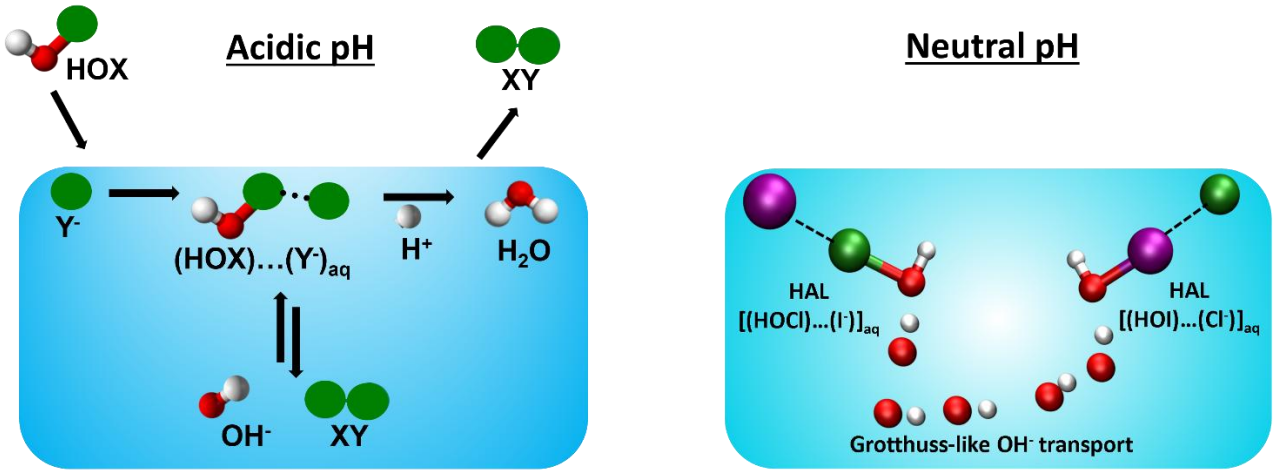


Figure 1 Dihalogen formation and halogen exchange mechanism at seawater

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Molecular Dynamics Insights into Charge and Mutation Effects in the Cytosolic Tail of LAMP2A: A Key Mediator of Chaperone-Mediated Autophagy

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The lipid environment has a major role in determining the structural and functional properties of transmembrane proteins[1]. In the selective protein degradation process known as chaperone-mediated autophagy, the oligomer of Lysosome-Associated Membrane Protein type 2A (LAMP2A) mediates substrate translocation and degradation. Although cytoplasmic tail histidine-to-alanine mutations are known to play a part in functionally disabling LAMP2A, the exact molecular mechanism underlying this is still unknown[2,3]. We perform 32 μs, all-atom molecular dynamics simulations of LAMP2A in a biologically relevant lysosomal membrane with different charges and cytosolic tail mutation to study this. Our analysis shows that the mutation stabilizes an α-helical structure, driving its insertion into the lipid bilayer, local membrane thickening, and increased helix tilt to accommodate hydrophobic mismatch. The alanine-containing mutant exhibits less protein-lipid interactions than charged versions. Additionally, simulations show decreased helix-helix interactions, which suggests a decrease in trimer stability. Destabilization results from the mutant's lack of important stabilizing interactions that are seen in charged systems at the residue level. All things considered, these results demonstrate how the mutation modifies the transmembrane protein's structural arrangement and dynamics.

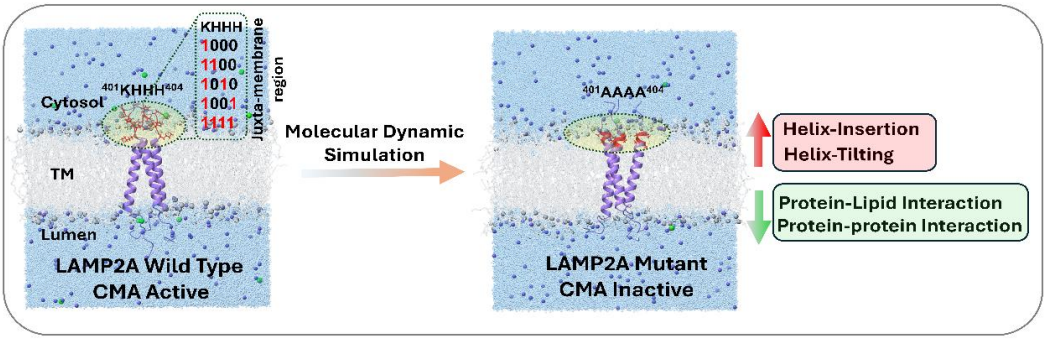


Figure 1 MD simulations (~32 μs) reveal that the CMA-inactive mutant disrupts membrane alignment via hydrophobic mismatch, causing residue burial, helix tilt, and weakened oligomer stability.

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Origin of Regioselectivity in Ru(II)-Catalyzed C−H Annulation of N-Chlorobenzamides with 1,3-Diynes

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Deciphering the reaction mechanism and the factors governing regioselectivity in transition metal-catalyzed C−H activation/annulation reactions with 1,3-diynes continues to be a compelling challenge. In this work, we conducted a detailed computational mechanistic investigation on a recently developed Ru(II)-catalyzed [4 + 2] annulation of *N*-chlorobenzamides with 1,3-diyne. The stepwise analysis of the reaction energetics indicates the migratory insertion step and the concerted reductive elimination/oxidative step to be the selectivity- and rate-determining steps, respectively. Finally, the distortion/interaction analysis suggests the steric effect as the determining factor for the observed regioselectivity for the formation of the 3-alkynylated product. Overall, the established insights into the catalytic mechanism and the origin of regioselectivity in the C−H activation/annulation reaction can be used as a guide to rationally design and develop novel transformation strategies for heterocycle synthesis.

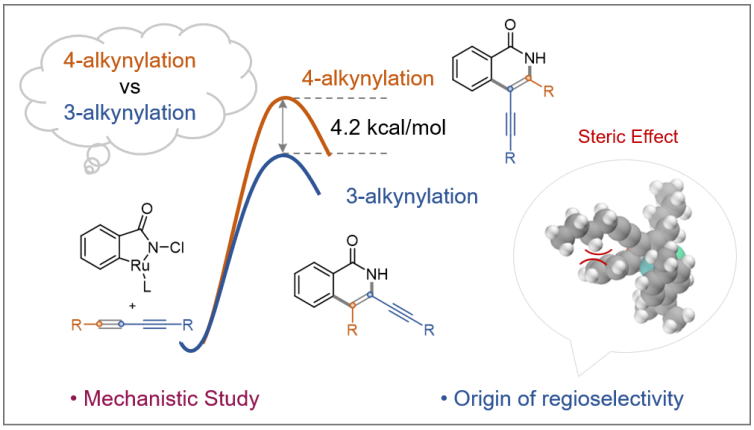


Figure 1. Origin of regioselectivity in Ru(II)-catalyzed C−H annulation reaction

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Towards the Selectivity and energetic of anti-Bredt Olefins – A Density Functional Theory Approach

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Anti-Bredt olefins (ABOs) are uncommon compounds featuring a double bond at the bridgehead carbon of small bicyclic systems, where pronounced geometric constraints hinder effective p-orbital overlap. Nevertheless, recent years have witnessed growing interest in synthesizing ABOs to harness their intrinsic strain energy. Advances in stabilization approaches and modern synthetic methodologies have further stimulated this renewed focus. Of particular note, a specific chemical precursor has recently been discovered that can produce an ABO as a transient intermediate[1]. The unique geometrical and electronic characteristics of these species open up alternative synthetic opportunities in medicinal chemistry and catalysis. In the present study, Density Functional Theory (DFT) is employed to systematically investigate the energetics, reaction mechanism, and structural determinants associated with ABO formation. Through detailed energy profiling, both thermodynamic stability and kinetic barriers are assessed to provide deeper insight into reaction feasibility. Altogether, this work advances the fundamental understanding of the molecular factors governing the formation, energetics, and stability of ABOs.

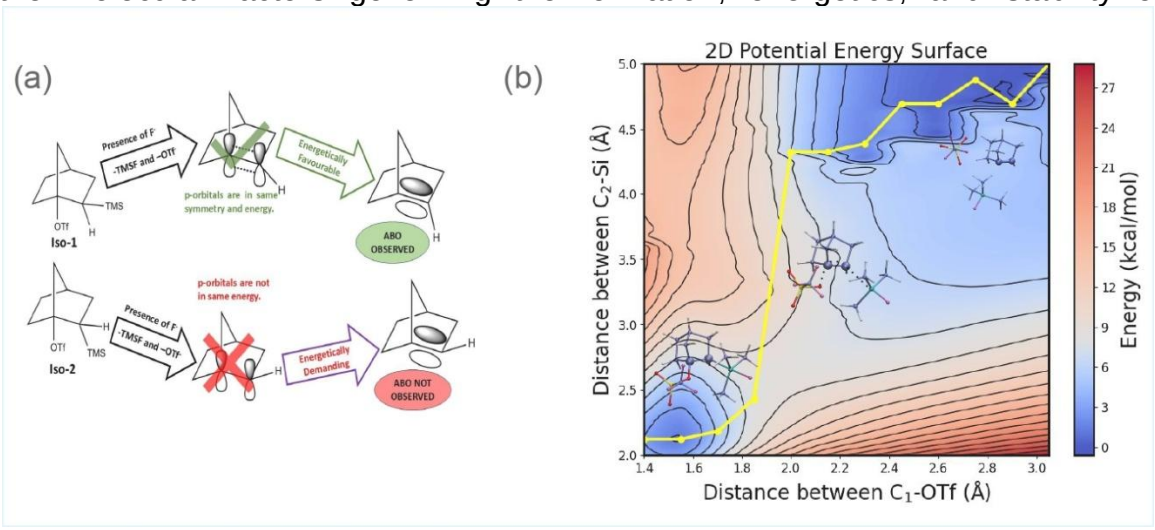


Figure 1 : (a) Both Iso-1 and Iso-2 can form an ABO in the presence of a fluoride source, but only Iso-1 has properly aligned p-orbitals that stabilize the bridgehead double bond, while Iso-2's misaligned orbitals create unfavorable energetics that prevent ABO formation. (b) The 2D potential energy surface scan reveals that ABO formation from Iso-1 proceeds via a concerted mechanism.

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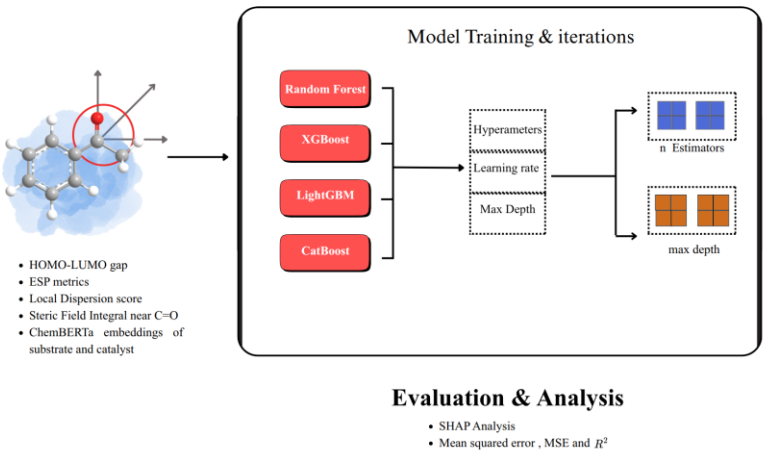
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Machine Learning Based Model Predict Enantiomeric Excess in arbonyl Reductions Using Hybrid Structure and Context Features

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We predict the enantiomeric excess of carbonyl reductions using a hybrid featurization that encodes the substrate and the catalyst. We opt for SMILES with ChemBERTa and we concatenate these learned embeddings with quantum based descriptors such as the HOMO to LUMO gap, electrostatic potential metrics, and a local dispersion score. We add steric descriptors such as Sterimol and a steric field integral near the carbonyl. We also include reaction context variables so additives and solvents are seen by the model alongside structure.We then train a suite of classical regressors to predict the enantiomeric excess . The base learners cover Random Forest, XGBoost, LightGBM, and CatBoost, and we also build a stacked ensemble with a Ridge meta learner that combines out of fold predictions from the base models. We sweep the number of trees in the Random Forest and select the best setting by cross validated error. The pipeline computes mean squared error and R^2 on validation and test and reports the mean and the standard deviation across seeds and folds. When synthetic augmentation is used, the synthetic samples are kept grouped with their parent reactions inside a single fold to avoid leakage. We also probe feature importance with SHAP style attributions so that steric, electrostatic, and dispersion terms can be linked back to chemical intuition and to guide condition selection.



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1. Machine Learning Based Model Predict Enantiomeric Excess in Carbonyl Reduction Reactions
J. Kaur, P. P. Singh, M. Jakhar, C. Dey, K. Thakran, R. Mayank, Shihan V C, S. Chakraborty* (Submitted)

Cotunneling Effects in the Geometric Statistics of a Nonequilibrium Spin-Resolved Junction

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Geometric or Pancharatnam-Berry phases[1], typically a property of adiabatic evolution in quantum systems, emerge as phase-like quantities in the nonequilibrium steady state of quantum transport. While geometric contributions to electronic transport in spinless quantum dots have been established for interacting systems[2], the role of cotunneling and spin-resolved transport remains underexplored. We investigate the role of cotunneling in the geometric statistics of a nonequilibrium spin-resolved quantum junction driven by phase-different adiabatic modulation of reservoirs' chemical potentials. We employed quantum master equations for a spin-resolved junction[3] with two spin orbitals coupled to electronic reservoirs. Using full counting statistics formalism, we numerically evaluated geometric flux contributions by tracking sequential tunneling, exchange cotunneling, and double charge-separated cotunneling processes separately for different system-reservoir coupling scenarios ($t_L \approx t_R$, $t_L \gg t_R$, and $t_L \ll t_R$) with and without Fock space coherences. For comparable coupling strengths ($t_L \approx t_R$), the sequential process dominates the total geometric flux when coherences are present. In the absence of coherences, cotunneling processes significantly contribute to the total geometric flux. The geometric flux exhibits a nonlinear dependence on the spin-spin interaction energy (U), contrasting with earlier findings for spinless systems. The cotunneling contribution to the total geometric flux can be made comparable to the sequential contribution by creating a right-sided asymmetrically stronger system-reservoir coupling strength. The nonlinear interaction energy dependence reveals distinct behaviour from spinless quantum dot systems, while asymmetric coupling enables tuneable cotunneling contributions. These findings establish cotunneling as a controllable mechanism for geometric phase manipulation in quantum transport devices.

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Relation between the free energy and d-band center- revisiting the HER descriptors

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Hydrogen fuel is considered as the cleanest renewable resource and the primary alternative to fossil fuels for future energy supply. Sustainable hydrogen generation is the major prerequisite to realize future hydrogen economy[1]. Noble metal-based electro catalysts are currently considered the most active materials for the hydrogen evolution reaction (HER). Noble-metal-based materials remain the most efficient HER catalysts. To fast screen HER candidates, most studies focus on descriptors like d-band center and Gibbs energy of H* adsorption on therotical perspective[2]. Most theoretical HER activity description focuses on the d-band center, defined as the average weighted energy of the d-band and can be applicable on explaining on metal centers. On the otherhand, binding strength of intermediate H*, and should be neither too strong nor too weak to achieve excellent HER activity, according to an empirical rule called the Sabatier principle[3]. The Gibbs free energy of H adsorption (ΔG_{H^*}) is a broadly used descriptor for the catalytic activity for HER. Specifically, zero free energy is optimal for HER performance. While ΔG_{H^*}can correlate with catalytic activity (e.g., a value near zero is optimal), however, Inability to capture dynamic changes in catalyst structure and chemical composition during operation, their limitations in explaining complex materials like Pt exist as a single-atom catalysts (SACs). On the other perspective, Platinum's surface reactivity towards H2O is still debated. DFT studies show that water dissociates more easily on Pt surfaces with low-coordinated atoms, where adsorption is stronger[4]. For efficient HER, an ideal catalyst needs a moderate d-band center to balance hydrogen binding strength. This ensures neither too strong nor too weak interaction with active sites[5]. At the atomic level, the understanding of the structure activity relationship still remains obscure in heterogeneous catalysis. Here we are going to do comprehensive detailed atomic level interaction analysis which provides fundamental insight into why platinum exhibits near optimal catalytic activity with the reported knowledge on descriptors. Moreover, for further studies we are going to give a new descriptor.

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Tunable Plasmonic - Metallic Cavity structure For High Performance Sensing

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Surface-Enhanced Raman Scattering (SERS) is a powerful tool for detecting and identifying molecules at ultra-low concentrations. Metallic nanostructures offer novel means of transforming free space light into local electromagnetic field in compact spaces[1,2]. Tailoring the confined EM field of the substrate of specific excitation wavelengths is an effective way to improve surface-enhanced raman scattering. In this work, we theoretically investigate the plasmonic performance of a nanocavitiy structures composed of gold (Au) and silver (Ag) on a SiO_2 substrate embedded within a sensing medium. Using finite element method we simulate a plasmonic nanostructure consist of a hollow cylinder, rectangular cavity and a crisscross structure to explore geometry dependent plasmonic effects. Optical response were analyzed in terms of absorption and extinction cross sections, which provide direct insights into the resonance conditions. In addition, electric field profiles were mapped at the resonance wavelengths, revealing intense hotspots localization at the cavities responsible for high electromagnetic field enhancement, enabling SERS effect. The Raman signal enhancement were further increased by systematically optimizing dimensions such as cavity width and introducing asymmetries in varied direction . Our results highlights that these hybrid Au-Ag/SiO_2 nanostructures provide versatile and stable plasmonic platforms with high sensitivity, suitable for SERS- based sensors.

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Water-Supercritical CO_2 Biphasic System for Efficient Extraction of Biomass Derived 5-Hydroxymethylfurfural (HMF)

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The use of biphasic systems has emerged as a prominent strategy to enhance 5-hydroxymethylfurfural (HMF) yields in acid-catalysed glucose conversion. While water-organic solvent biphasic systems have demonstrated promising efficiency, concerns regarding the environmental impact of organic solvents and the use of mineral acids remain significant[1,2]. To address these issues, we explore a greener alternative based on a water-supercritical carbon dioxide ($scCO_2$) biphasic system. In this setup, the in-situ formation of carbonic acid at the water-$scCO_2$ interface eliminates the need for external acid catalysts, making the system more environmentally benign[3,4]. However, despite its green credentials, the water-$scCO_2$ system has shown limited ability to match the HMF extraction performance of conventional organic solvent systems. In this study, we systematically investigate the influence of temperature, pressure, and salt concentration on HMF extraction in the water-$scCO_2$ biphasic system. Classical molecular dynamics (MD) simulations using GROMACS were employed to understand the interfacial behaviour and key molecular interactions that govern HMF partitioning. Our findings reveal the optimal conditions for efficient HMF extraction, highlight the structural and dynamic features of the water-$scCO_2$ interface, and elucidate the role of dissolved salts in modulating interfacial properties and solute transfer.

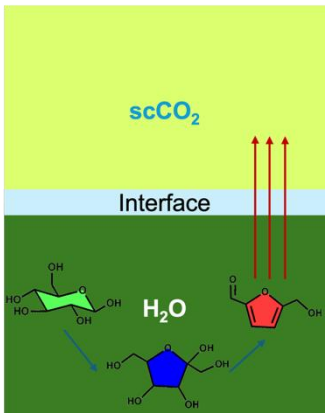


Figure 1 Schematic representation of HMF extraction on H_2O-$scCO_2$ biphasic system.

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SymbolicCI: An *Ab Initio* Framework for Modeling Biexcitons in Molecular Aggregates

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Understanding biexcitonic phenomena in molecular aggregates is crucial for designing next-generation optoelectronic and energy-harvesting materials.[1] We introduce a unifying *ab initio* framework for analyzing biexcitonic states using a novel symbolic configuration interaction method, ***SymbolicCI***.[2] This yields adiabatic states in a (quasi-)diabatic basis, aiding the study of photophysical processes. ***SymbolicCI*** enables large-aggregate modeling through fragmentation, overcoming the size limits of conventional wavefunction-based methods. This supports both transparent excited-state analysis and systematic biexciton tuning for materials design.

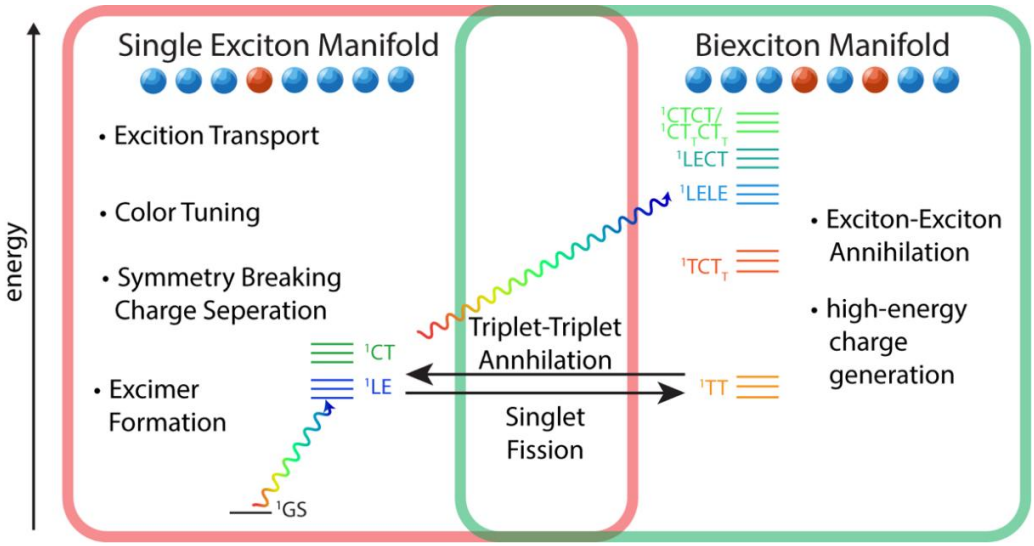


Figure 1 Scheme illustrating the energetic ordering of the one-particle exciton and the biexciton manifold and processes connected to these manifolds.

The method clarifies the classification, energetic hierarchy, and couplings of biexcitons formed from local excitation (LE), charge-transfer (CT), and triplet (T) states. We study ^{1}TT, ^{1}LELE, ^{1}LECT, ^{1}TCT, ^{1}CTCT, and ^{1}CT$_T$CT$_T$ states within the singlet manifold. Benchmarking against non-orthogonal configuration interaction (NOCI)[3] for stacked ethene and anthracene shows strong agreement — especially for LE-based states — while offering a clear framework for biexciton mixing and coupling. We find ^{1}LECT states are close in energy to ^{1}LELE, making them key low-lying configurations. In contrast, ^{1}CTCT and ^{1}CT$_T$CT$_T$ states lie significantly higher. Our approach aims to deepen understanding of biexcitonic processes such as exciton-exciton annihilation and high-energy charge generation.

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Theoretical Chemistry Symposium
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Mapping the Molecular Mechanism of Zinc Catalyzed Suzuki-Miyaura Coupling Reaction: A Computational Study

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The Suzuki-Miyaura Coupling (SMC) reaction creates carbon-carbon bonds and is widely used across various fields. Palladium, the traditional catalyst, is expensive, toxic, and scarce. Zinc provides a cheaper, environmentally friendly alternative but lacks detailed mechanistic understanding. This study employs computational methods to investigate zinc's role and enhance reaction efficiency. It identifies a four-coordinate Zn (II)-DMEDA complex as the active catalyst for zinc-catalyzed Suzuki-Miyaura Coupling, ruling out the formation of Zn (0) species due to high energy costs. Unlike typical oxidative addition-reductive elimination pathways, the reaction proceeds via a redox-neutral mechanism involving an initial transmetalation step followed by concerted nucleophilic substitution and reductive elimination. The rate-determining step, the activation of the alkynyl halide, has an energy span of 27.2 kcal/mol, matching the experimental reaction temperature of 80°C. Computational analyses confirmed the stability of intermediates, including the aryl zincate complex, and dismissed radical pathways due to unfavorable energetics. These insights open the door for sustainable synthesis of functional organic scaffolds using zinc as an eco-friendly catalyst.

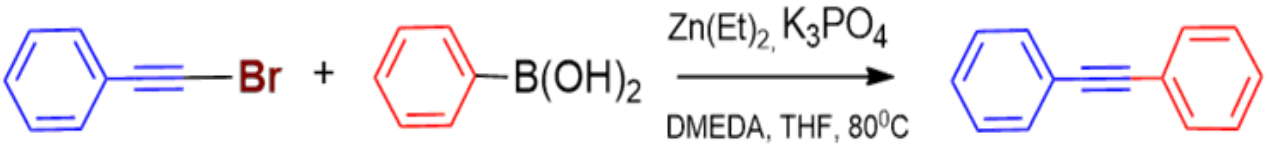


Figure 1 Model Reaction Mechanism for Zinc-Catalyzed Suzuki-Miyaura Coupling

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Theoretical Chemistry Symposium
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Molecular Recognition of Water Pollutants through IR and NMR Spectroscopy

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Water pollution has become a significant threat to marine life and human health, with benzene diols and polyaromatic hydrocarbons (PAHs) being the major pollutants.[1, 2] Thus, detecting and removing them from water remains a scientific challenge. In our work, we have taken the sulfur analogue of the "Green Box"[3, 4] (DiS) as the host for the recognition of pollutants (catechol, resorcinol, hydroquinone, naphthalene, anthracene, and phenanthrene), with spectroscopic techniques, infrared (IR), and nuclear magnetic resonance (NMR). The goal was achieved by integrating classical molecular dynamics (MD) simulations, quantum mechanical calculations, and a hybrid quantum mechanics/molecular mechanics (QM/MM) approach. An in-depth investigation of the IR and NMR spectra rationalises the observed shifts in the host-guest complexes, which eventually are their "fingerprints". We hope the systematic study will help the scientific community to use the spectroscopic methods in the molecular recognition of water pollutants.[5]

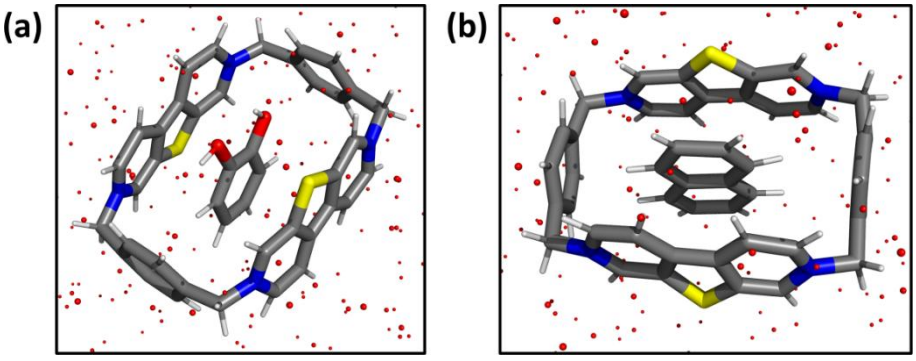


Figure 1. The post-MD simulation structures of DiS complexes with **(a)** catechol and **(b)** naphthalene, in water.

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Theoretical Chemistry Symposium
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Short-range 2c-2e resonance integrals for $^1\Sigma$ states utilizing H-like s-orbitals as basis set

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The evaluation of resonance integral of (2c-2e) molecular scaffold engraved a longstanding challenge within electron structure theory. The interactions among electron-electron (e-e) and electron-nucleus (e-n) engender substantial obstacles in Schrodinger's Equation. In contrast to Slater type orbitals (STO), (2l+2)-Associated Laguerre, Gaussian type orbitals (GTO), B-spline and Sturmian functions, H-like basis set exhibit generic radial nodes that represents formidable obstructions in separating electronic and nuclear coordinates in Coulomb as well as resonance integrals. Since, the advent of angular nodes poses a fundamental challenge for both bound and unbound H-like orbitals, thereby necessitating the development of analytical expressions for resonance integrals from the outset of study. The Coulomb (J) and resonance (K) integrals of small 2c-2e framework were analytically straightened out by employing Coulomb Green function, elliptic coordinates, Sheffer identity, and Lah number functions tailored to H-like s-orbitals. We have adopted a framework that incorporates e-e, e-n and n-n interactions for $^1\Sigma$ molecular states representing as the closed forms of resonance and overlap integrals (S) in the context of Born-Oppenheimer (BO) approximation for a small 2c-2e molecular scaffold parameterized by bond characteristics. To simplify the analysis, we have focused on H_2 molecule.

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Ligand-Driven Hot-Carrier Dynamics in Metal-Rich CdSe Quantum Dots: Insights from First-Principles and Nonadiabatic Molecular Dynamics

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Hot-carrier dynamics critically determine the optoelectronic performance of semiconductor quantum dots, with direct implications for next-generation photovoltaics and photocatalysts. Here, we examine how halide ligands—fluorine, chlorine, bromine, and iodine—modify the structural, electronic, and non-radiative relaxation properties of cadmium-rich CdSe quantum dots $Cd_{35}Se_{20}X_{30}$. Using a combined approach of density functional theory (DFT) and nonadiabatic molecular dynamics (NAMD) within the PYXAID framework, we construct atomistic models to probe carrier relaxation processes.

Our results reveal that ligand chemistry exerts a strong influence on bonding geometry, band gaps, and nonadiabatic couplings (NACs), which together dictate carrier lifetimes. Bromine-passivated quantum dots show the most favorable behavior, with extended hot-carrier lifetimes arising from reduced NAC strengths and moderate conduction band gaps that slow relaxation. In contrast, chlorine passivation leads to the fastest relaxation due to enhanced NAC and narrower band gaps.

These findings highlight bromine as a promising surface ligand for prolonging carrier lifetimes and demonstrate the potential of rational ligand engineering to optimize quantum dot–based optoelectronic devices.

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Pushing the Boundaries of Pnictogen-Bonding Organocatalysis: A Clash of Sb(III) versus Bi(III)

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The σ-hole-mediated noncovalent organocatalysis involving the pnictogen (Pn) elements has thus far been explored mostly from nitrogen to antimony, with antimony identified as the most effective catalyst. Herein, density functional theory calculations have been carried out to demonstrate that tri-aryl (Ar)-substituted bismuth(III) complexes can outperform their antimony counter-parts in both anion (Cl) binding and catalytic activity. Using a range of computational methods, a good correlation between the σ-hole strength, chloride binding affinity, and the reaction barrier is established. Notably, the findings reveal that dispersion interactions are the dominant force in catalysts with weaker σ-holes, while electrostatic interactions prevail in catalysts with stronger σ-holes (for the anion abstraction step). In all cases,Bi(III) catalysts emerge as the winner over the Sb(III) analogues.Additionally, beyond the primary Pn…Cl interactions, several secondary interactions such as Cl…H/F—C(Ar) and Cl…H—C(Si-TBS) also play a significant role in stabilizing the transition states.[1]

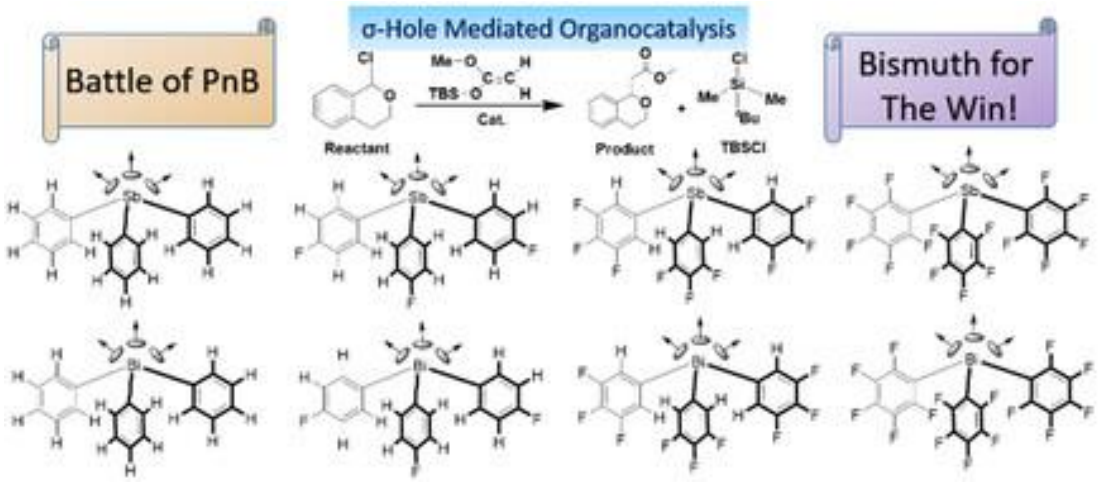


Figure:-Tri-aryl-substituted bismuth(III) complexes exhibit superior anion (Cl−) binding affinity and perform as a better organocatalysts as compared to their antimony analogues. Additionally, the impact of increasing fluoride substitutions on the aryl groups is explored, with a focus on how these substitutions affect the electronic structure of these organocatalysts, strength of the σ-holes, Cl− binding, and the reaction barrier.

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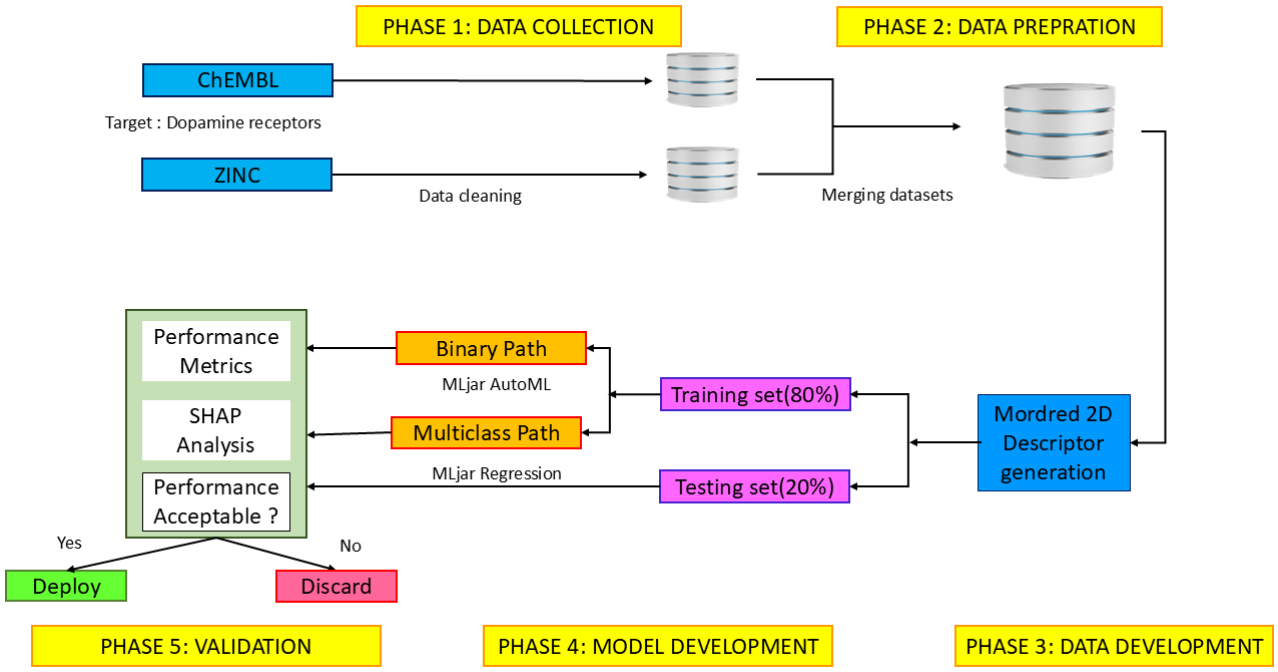
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Ligand-Centered Machine Learning for Dopaminergic Activity and Receptor Subtype Selectivity

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Dopaminergic signalling depends on a heterogeneous family of receptors DRD1–DRD5, and transport/metabolic proteins that regulate extracellular dopamine. we describe a ligand-based machine-learning approach to differentiate compounds that exhibit measurable dopaminergic activity and privilege receptor subtype selectivity, based exclusively on two-dimensional molecular descriptors. In this work, records were aggregated from multiple bioactivity repositories, harmonized across identifiers, de-duplicated, and standardized at the target level to ensure data quality and consistency. The resulting dataset captured both agonists and antagonists across receptor families, enabling the development of a balanced model. The models generalized well to held-out compounds and highlighted physicochemical and graph-topological properties as salient determinants of activity, with selectivity signatures distinguishing major receptor families. Furthermore, analysis of feature importance suggested that molecular polarity, aromaticity, and connectivity indices play critical roles in shaping subtype-specific binding profiles. Taken together, these results demonstrate that simple descriptor-driven machine learning approaches can effectively capture complex structure–activity relationships in dopaminergic systems, providing a scalable framework for prioritizing chemical matter in early-stage drug discovery in the future.

Figure: Overview of the workflow.



Tuning Spintronic Properties of 2D OsC Monolayers with 3d Metal Functionalization: A First-Principles Study

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Magnetic materials, driven by collective electron spin interactions, are vital for spintronics, quantum devices, data storage, and sensing. Here, we report a first-principles study of 2D OsC monolayers functionalized with 3d transition metals (TMs: Sc, Ti, V, Mn, Fe, Co, Ni, Zn) using density functional theory (DFT) with spin-orbit coupling (SOC). Pristine OsC is non-magnetic and metallic, as shown by its band structure [Fig. 1(a,b)]. TM adsorption induces significant electronic and magnetic changes. Adsorption energies confirm strong chemisorption, and cohesive energies indicate high stability. Spin-polarized density of states (DOS) reveals that Sc, Ti, Fe, Co, Ni, and Zn induce ferromagnetic (FM) states, while V and Mn yield antiferromagnetic (AFM) ordering. Notably, the Mn-adsorbed OsC monolayer is promising for spintronics due to its strong magnetic ordering and moments [Fig. 1(c,d)]. These results demonstrate TM-functionalized OsC monolayers as a tunable platform for advanced spintronic and magnetic devices.

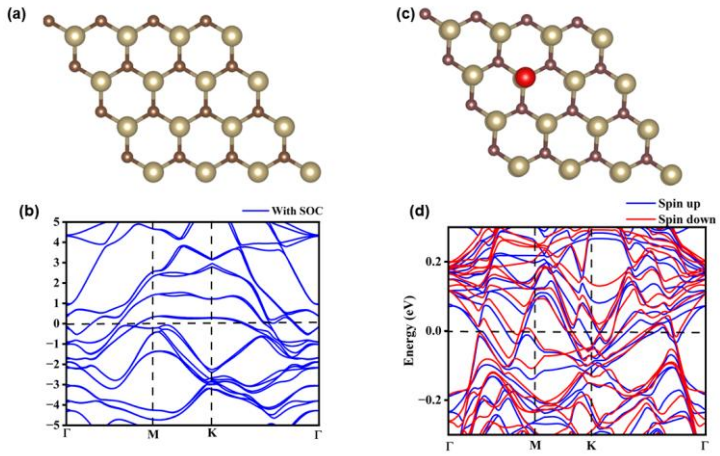


Figure 1 (a) optimized structure of pristine OsC, (b) band structure of pristine OsC, (c) optimized structure of Mn-adsorbed OsC, and (d) band structure of Mn-adsorbed OsC.

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Theoretical Chemistry Symposium
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Quantum Chemical Insights into Lewis Acidity and Electronic Structure of 1,2,3-Triazolium Ions

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Nitrogen-centered cations play key roles in medicinal chemistry and catalysis. Among them, nitrenium ions (R–N^+–R) and nitreones (L→N^+←L) represent two distinct electronic classes that differ in bonding and lone-pair distribution at the central nitrogen. Their cyclic counterparts — cyclic nitrenium ions (CNIs) and cyclic nitreones (CNTs) — have attracted significant attention due to their enhanced stability and versatile applications. In particular, cyclic five-membered 1,2,3-triazolium ions (CFTIs) form an important subclass of CNIs. These species display electrophilic, rather than nucleophilic, behavior (unlike *N*-heterocyclic carbenes) and are employed in Lewis acid catalysis, photocatalysis, and even biological systems.

In this study, a systematic quantum chemical investigation was performed on CFTIs with substitutions at N^1/N^3/C^5 and their fused derivatives (benzofused and *f*CFTIs). Key electronic descriptors such as hydride ion affinity (HIA) and the global electrophilicity index (ω) were evaluated to quantify Lewis acidity and electrophilicity. Complexation enthalpies with model Lewis bases (PMe_3 and 1,3-dimethylimidazoyl-2-ylidene (NHC)) showed a strong correlation (R = 0.99) between ΔH_{PMe_3} and ΔH_{NHC}, establishing a reliable predictive metric to predict Lewis acidity.[1]

Benzofusion led to a moderate increase in Lewis acidity, whereas fusion across the N^1–C^5 and N^3–C^4 bonds (*f*CFTIs) resulted in the decrease of Lewis acidic character. Interestingly, fusion across both bonds allowed exploration of the CNI and CNT characters within a single molecular framework.[2] These findings elucidate the electronic features governing Lewis acidity in CFTIs and offer insights for tuning reactivity of CFTIs.

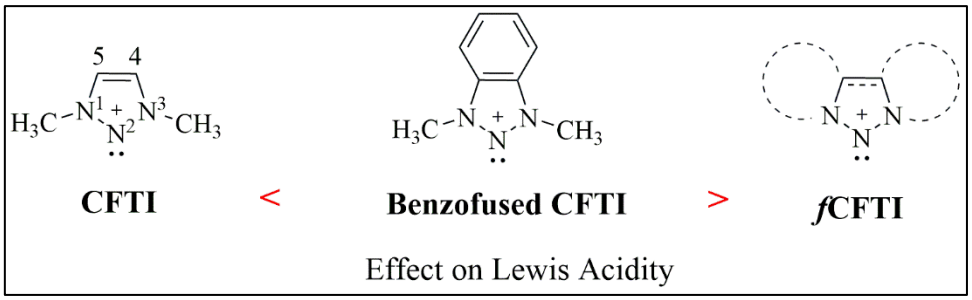


Figure 1. Quantum chemical analysis on effect of ring fusion on Lewis acidity of CFTIs**.**

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Dissecting the Binding Energetics of EGFR complexes Using Fragment Molecular Orbital method

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Experimental methods for determining protein-ligand binding affinities are often slow and expensive, limiting the pace of drug discovery. Computational approaches, in conjunction with experiments, can provide a faster and most cost-effective alternative, enabling researchers to explore a broader range of potential drug candidates.[1] However, the accuracy of computational methods vary depending on the methodology and complexity of the systems. This study focuses on the Epidermal Growth Factor Receptor (EGFR), which is crucial for the progression of Pancreatic Ductal Adenocarcinoma (PDAC) and lung cancer, making it a key target for therapeutic intervention.[2] The binding energetics of four EGFR inhibitors—Erlotinib, Gefitinib, Afatinib, and Osimertinib—were analyzed using the Fragment Molecular Orbital (FMO) method with Pair Interaction Energy Decomposition Analysis (PIEDA). MP2-level calculations provided a more accurate description of noncovalent stabilization, showing Osimertinib with the strongest computed interaction (–99.0 kcal/mol). Experimentally, Erlotinib (–10.72 kcal/mol) and Gefitinib (–10.57 kcal/mol) exhibited similar affinities, Afatinib showed moderate binding (–9.97 kcal/mol), and Osimertinib appeared weaker (–8.77 kcal/mol) due to its irreversible mechanism. Residue-level analysis revealed that electrostatics dominate binding, mainly through acidic (GLU211, ASP201, GLU177) and basic residues (LYS044, LYS019, LYS111), with additional dispersion and charge-transfer effects from hydrophobic and aromatic residues (TRP185, TYR196, LEU212). The consistent ranking of key residues across methods confirms the robustness of the interaction profiles. Overall, FMO–PIEDA effectively links total binding energetics with residue-level contributions, offering insights for designing next-generation EGFR inhibitors.

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Theoretical Chemistry Symposium
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Tetracarbonyls of alkaline earth metals: Preference towards square pyramidal geometry and d-orbital π-backbonding

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Traditionally, alkaline earth metals form compounds using valence *ns* and *np* orbitals. The first report on octacarbonyls of alkaline earth metals $M(CO)_8$ (M = Ca, Sr, or Ba) questioned the traditional bonding concept.[1,2] The detailed experimental and theoretical studies suggest that *d* orbitals of alkaline earth metals actively participate in bonding with carbonyl groups. Here, we conducted a detailed computational quantum mechanical study to explore the role of *nd* orbitals in influencing the geometry of tetra-carbonyl alkaline-earth metals, $M(CO)_4$, (M = Mg - Ba). Four stationary points are possible for $Mg(CO)_4$, whereas seven or eight were identified for the heavier analogues (Figure 1). All tetra-carbonyls have ten total valence electrons. The two extra valence electrons mainly occupy the CO π* orbitals in all $Mg(CO)_4$ isomers. The most stable isomer of $Mg(CO)_4$ adopts a square-pyramidal geometry, which can be attributed to the reduced *s* orbital contribution of Mg in σ-bond formation. This geometry also reduces the diffuseness of the *3p* orbital by forming a *sp* hybrid orbital for efficient overlap with the CO π* orbital. In contrast, the extra two valence electrons in $M(CO)_4$ (M = Ca - Ba) occupy the valence *nd* orbitals. The larger number of isomers for the heavier analogues can be attributed to the possible distribution of these two valence electrons among five *d* orbitals. Square-pyramidal geometry promotes strong backdonation of the d_{xy} and hybridized $sp_zd_z^2$ orbitals of heavier alkaline earth metals to the CO π* orbital, compared to square-planar, see-saw, and tetrahedral geometries. The thermodynamic stability of the tetracarbonyls of alkaline earth metals is relatively low (2.1 - 7.8 kcal/mol) compared to heavier analogues (16.6 - 33.8 kcal/mol in $Ca(CO)_4$, 11.3 - 27.8 kcal/mol in $Sr(CO)_4$ and 22.0 - 38.3 kcal/mol in $Ba(CO)_4$), as indicated by dissociation energies. The higher thermodynamic stability of the heavier $M(CO)_4$ complexes is due to electron backdonation from *d* orbitals to the CO π* orbital. Electron redistribution among different *d*-orbitals leads to multiple isomeric structures.

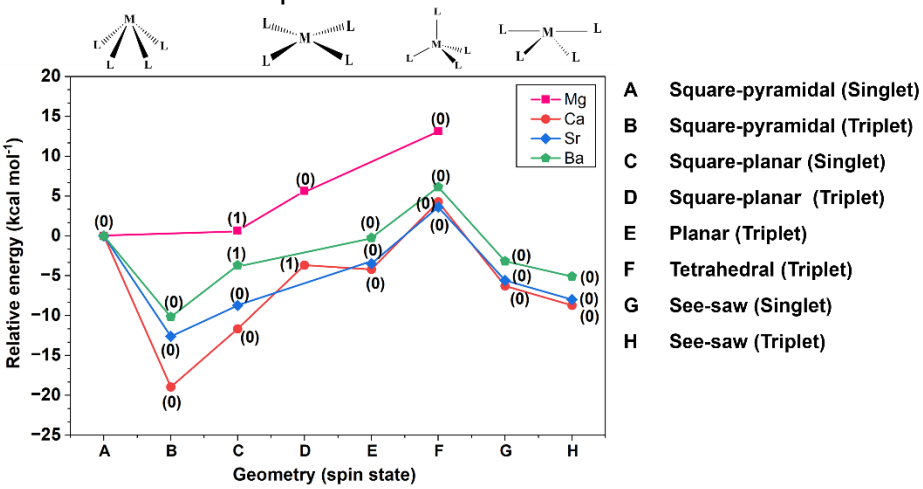


Figure 1: Relative Energies (in kcal mol^{-1}) along with their geometry and spin state of various isomers of $M(CO)_4$, (M = Mg - Ba), calculated using the M06/def2-TZVPP//BP86/def2-TZVPP level of theory. The numbers of imaginary frequencies are given in parentheses.

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Machine Learning Insights to Predicting Spillover Potential of Animal Viruses Infecting Humans

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Emerging outbreaks often start when viruses jump between hosts, but defining the host range of novel viruses remains challenging. We present a protein-focused machine-learning approach that assigns a Host Spillover Prediction (HSP) score to viral sequences, estimating their likelihood of infecting humans. Using receptor-binding proteins of animal infecting viruses, our analysis highlighted elevated spillover signals in H1N1 influenza, HKU5-related coronaviruses, and Nipah-related viruses. Benchmarks demonstrate strong accuracy and generalizability, even with limited training data. By converting protein sequences into a biologically interpretable risk metric, this approach provides a scalable, actionable early-warning tool to prioritize animal viruses for surveillance and rapid response.

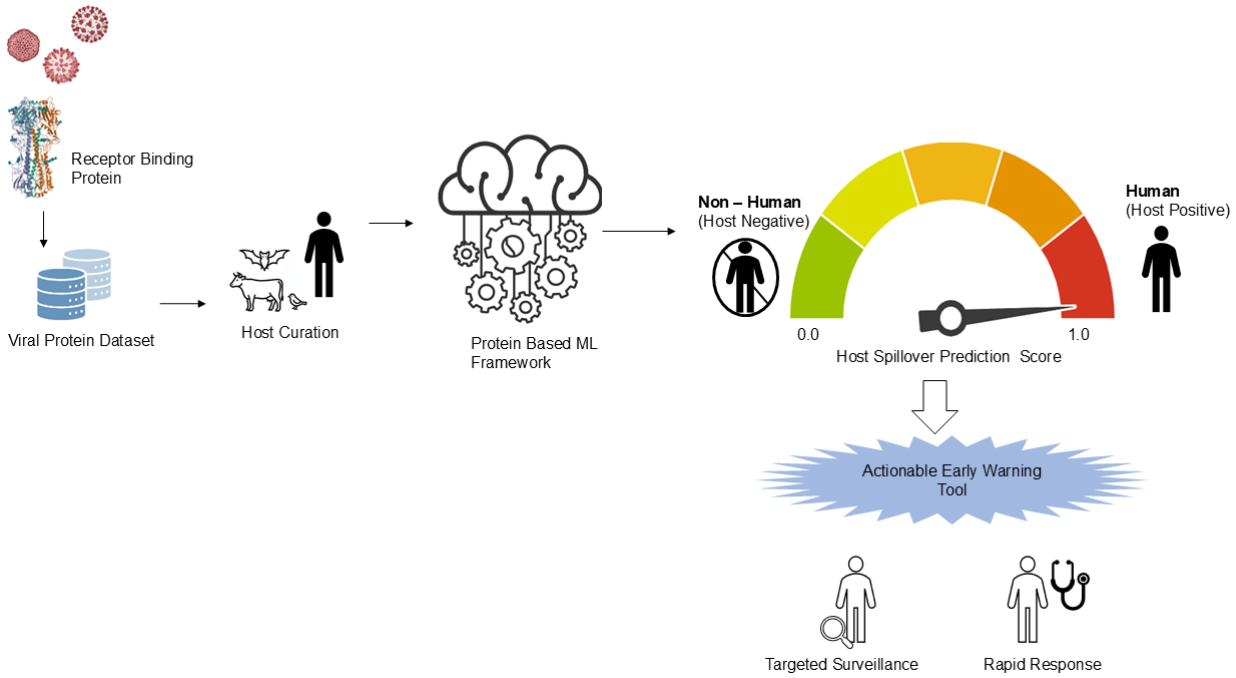


Figure 1 Schematic overview of the protein-based machine learning framework for host spillover prediction in animal viruses. Viral protein datasets are curated and analyzed to assign a Host Spillover Prediction (HSP) score, distinguishing non-human from human infection potential, thereby enabling actionable early-warning tools for targeted surveillance and rapid response

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Structure and Dynamics of Cyclic alkyl ammonium amino acid based Ionic liquids for CO_2 capture: A combined DFT and MD study

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Amino acid based ionic liquids (AAILs), and in general ionic liquids, have emerged as versatile solvents for numerous applications, including gas capture[1]. In this study, we have investigated several AAILs consisting of Cyclic alkyl ammonium (Pyrrolidinium $[Pyr]^+$ and Piperidinium $[Pip]^+$) cations and amino acid anions[2,3], to explore CO_2 absorption mechanisms and dynamics. The structural organization, cation-anion Hydrogen Bond (HB) interactions were systematically investigated using DFT calculations along with Atoms in Molecules (AIM) analysis. The CO_2 absorption by the AAILs leading to the formation of carbamic acid showed the lowest activation barrier for the [Pyr][His] system [Figure 1(a)]. MD simulations provide insight into the transport and dynamic properties. The density profile curves showed a preferential accumulation of CO_2 at the CO_2/AAIL interface following the trend [His] > [Arg] > [Lys] for a given cation [Figure 1(b)]. The [Pyr][Lys] and [Pip][Lys] systems showed faster dynamics, consistent with higher diffusion and ionic conductivity. The self-diffusion coefficients of ions increase, while the bulk densities of AAILs remain almost constant upon CO_2 binding. Additionally, the ether functionalization of the cation is also explored.

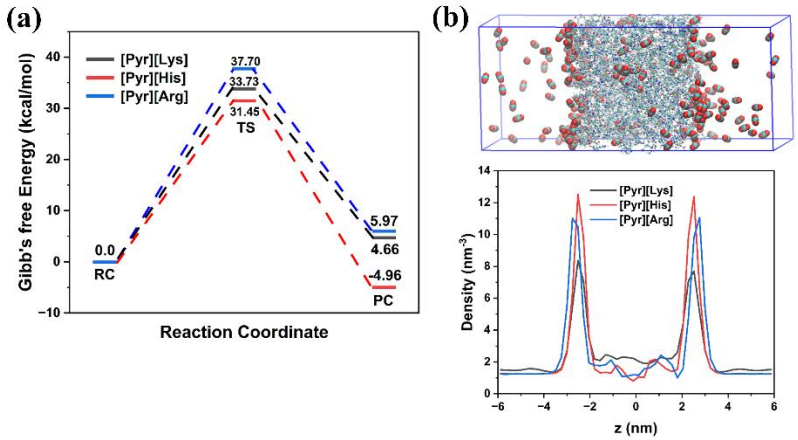


Figure 1. (a) The Gibbs free energy, and (b) Density profile Diagram for the studied AAILs.

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Rheological and Dynamic Properties of the Water-in-KCl System

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Understanding the **"**water-in-ions" regime—where ions are the majority species and water exists as a minority component—has become increasingly significant across energy, environmental, and materials research**.** In this ion-rich or water-deficient regime, water molecules are strongly coordinated by ions, giving rise to unique rheological, structural, and dynamic properties that differ markedly from those of ordinary aqueous solutions. However, probing water dynamics in such highly concentrated electrolyte systems remains a major experimental challenge[1]. Researchers have turned to molecular dynamics simulations to study the properties of such systems[2,3].

To gain deeper insights, we performed molecular dynamics simulations of potassium chloride (KCl) with SPC/E water model under ambient conditions. The mean-squared displacement of water molecules reveals three distinct regimes**:** (i) a short-time ballistic regime, (ii) an intermediate subdiffusive regime, and (iii) a long-time diffusive regime. This contrasts with conventional aqueous solutions, which typically show only the ballistic and diffusive regimes. The transitions between these regimes were further analyzed using non-Gaussian parameters**,** confirming the presence of dynamical heterogeneity in the ion-rich environment.

We also computed the shear viscosity, which increases sharply with ion concentration. The concentration dependence of viscosity was well described using an empirical relation that extends the Jones–Dole equation. Furthermore, analysis of the dynamic moduli in the GHz–THz frequency range reveals that the loss modulus (G″) dominates at low frequencies, while the storage modulus (G′) overtakes at higher frequencies, indicating a transition toward solid-like behavior**.** Interestingly, pure water exhibits a qualitatively similar crossover at high frequencies[4].

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Mechanistic Insights into Shape-Selective Molecular Recognition through Rotational Dynamics in MOFs using Ab-initio molecular dynamics

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Metal-organic frameworks (MOFs) are compounds composed of metal ions or clusters coordinated to organic linkers, forming a framework with high crystallinity, substantial porosity, and extensive surface area. Owing to their very low density, MOFs exhibit highly dynamic structures (localized and global), in contrast to other crystalline materials that possess restricted structural mobility. This dynamic nature is very important for selectivity and adsorption capacity. Given the widespread application of MOFs in adsorption, gas separation, and catalysis, it is imperative to investigate how structural dynamics influence the interactions between the framework and guest molecules. A strong correlation has been observed between the dynamics of the linkers and host-guest interactions, with each exerting a significant influence on the other. Though, experimental methods like pulsed filed gradient NMR and IR microscopy can be used to understand adsorption and diffusion process in MOF, microscopic events during diffusion in flexible MOFs are challenging to comprehend. Here, we have explored molecular dynamic simulations to understand the chemical isomer diffusion selectivity in selected MOFs, as illustrated below.

This poster presents an investigation into the influence of local rotational dynamics on the interactions between framework and guest molecules. Specifically, a pillared-layer structure featuring PCU topology with the chemical composition $Cu_2(L_{Dyn})_2DABCO$ (where LDyn denotes either bicyclo[2.2.2]octane-1,4-dicarboxylic acid or 1,4-benzenedicarboxylic acid, and DABCO refers to 1,4-diazabicyclo[2.2.2]octane) has been examined. Within the PCU topology, the two observed MOFs, differentiated by their linkers exhibit distinct rotational dynamics and barriers. The specific rotational barriers of the linkers enable the distinction of branched isomers. Although the kinetic diameters of 2,2-dimethylbutane (~6.2 Å) and 2,3-dimethylbutane (5.6 Å) are quite similar, an inverse trend is observed. The bicyclo linker demonstrates a preferential recognition for 2,2-DMB, which possesses the larger kinetic diameter. These specific interactions manifest as changes in localized linker dynamics, quantifiable through dihedral angle measurements. Notably, the bicyclo linker exhibits distinct dihedral angles in the presence of adsorbate molecules, whereas the BDC linker does not display a comparable trend. This phenomenon was subsequently corroborated by the isosurface density plots of guest molecules inside framework derived from ab initio molecular dynamics (AIMD) trajectories. These reveals a clear diffusion pathway for 2,2-DMB within the bicyclo MOF.

A similar trend can be observed in the UiO-67 structure with an Fm3m topology, where linker dynamics exhibit a significant difference between the presence and absence of specific guest molecules, resulting in specific interactions. We propose that localized linker dynamics can be studied to investigate interaction sites and predict selectivity before performing an adsorption experiment.

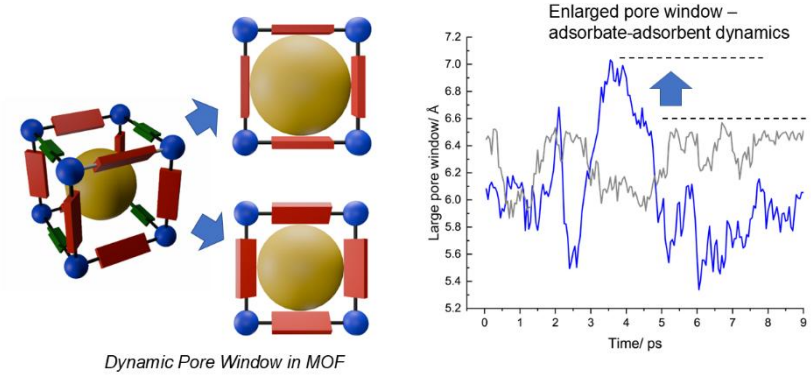


Figure 1 Schematic representation of linker dynamics in MOFs affecting pore window size (left) and larger pore window diameter vs time plot of $Cu_2(bicyclo)_2DABCO$ in presence of 2,2 DMB (blue) and in absence of 2,2 DMB (grey) computed from AIMD trajectory (right)

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Insight into electrochemical formic acid oxidation reaction on different PtBi and Pd anchored PtBi facets– a first-principles study

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The electrochemical formic acid oxidation reaction (FAOR) is crucial for direct formic acid fuel cells (DFAFCs), which are portable power sources. Additionally, FAOR is studied for hydrogen production and electrochemical sensors, having low CO poisoning compared to other small organic molecule oxidations. FAOR typically proceeds through a dual-path mechanism involving either a direct pathway with CO_2 formation or an indirect path with CO, electrons, and protons formation at the anode. Generally, the high desorption energy of CO from the metal surfaces disfavors the indirect path; hence, an efficient catalyst should have high selectivity towards the direct path of FAOR. Recent experimental studies have shown that PtBi is a promising catalyst for FAOR.[1] In this study, we investigate both the direct and indirect pathways of FAOR using the computational hydrogen electrode model (CHE).[2] Our results suggest that the direct path of FAOR is more feasible than the indirect path in PtBi (111), PtBi (110), and PtBi (100) facets. All possible conformations of different intermediates with electronic insights are explicitly studied. After the addition of Pd, Pd@PtBi is a more efficient FAOR catalyst via the direct path. We establish a correlation of the absorption energy of formic acid, the desorption energy of CO_2, the d-band center of the catalyst, and the onset potential via DFT study. We believe the understanding of proper binding sites, reaction paths, and mechanistic, electronic insights will play an essential role in optimizing catalytic efficiency.

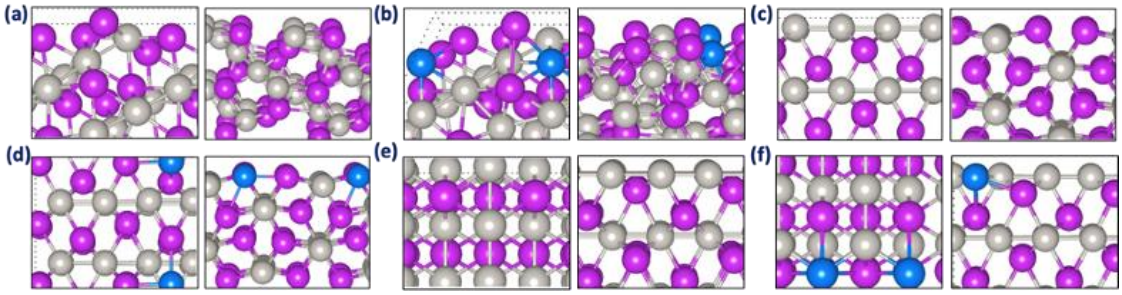


Figure 1. Represent different structures of different faces (left, top view, and right, side view) of (a) PtBi (111), (b) Pd@PtBi (111), (c) PtBi (110), (d) Pd@PtBi (110), (e) PtBi (100), and Pd@PtBi (100). White, pink, and blue represent Pt, Bi, and Pd, respectively.

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EFFECTS OF ELECTRON-WITHDRAWING AND DONATING GROUP SUBSTITUENTS ON DIAZIRINE: AN EXCITED STATE NON-ADIABATIC MOLECULAR DYNAMICS STUDY.

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Photolysis of diazirine from an excited state proceeds via the conical intersection (CI) and avoided crossings. These crossings promote the formation of products in the ground electronic state. When two or more electronic states have nearly equal or equal energies, it results in coupling between the electronic states and nuclear motions and hence the Born-Oppenheimer approximations break down at such junctions.[1] These couplings provide opportunities for the excited molecule to reach the ground state via the narrow-shaped channels in a radiation-less manner. Such an overall process is called a non-adiabatic phenomenon.[2] In this study, the initial dynamics for diazirine and its substituted derivates were started at n-π* excited state at the S1 level and predictably the molecule hops back into the S0 ground state after a certain period. Such a process occurs via a non-adiabatic mechanism and the products yielded are molecular nitrogen and carbene. We have characterized four diazirine systems, those are 1) unsubstituted diazirine CH2N2 (DAZ), 2) fluoro-diazirine CHFN2 (FDAZ), 3) methoxy-diazirine CH(OMe)N2 (MDAZ) and 4) fluoromethoxy-diazirine or push-pull diazirine CF(OMe)N2 (PPDAZ).[3] These four systems have been chosen in such a way that it enables us to have a distinct comparative study among the substituents that have electron-withdrawing effect (EWG), i.e., fluorine and electron-donating effect (EDG) i.e. methoxy and effects of both the EWG and EDG i.e. push-pull effect on diazirine.[4]

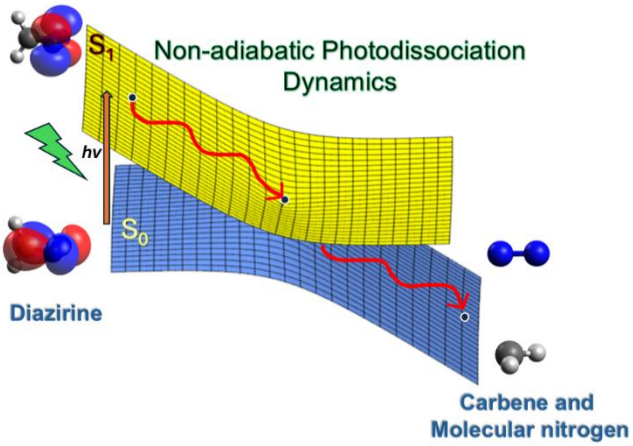


Figure 1 Schematic of Diazirine photolysis.

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Theoretical Chemistry Symposium
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Transition state model for the chemical hydrogen battery

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Transition state modeling is a powerful tool for unraveling the mechanistic intricacies of chemical reactions. It plays a pivotal role in the design of new catalytic systems, facilitating progress in the field of catalysis.[1] A carbon-neutral chemical hydrogen battery is the most sustainable approach for the storage and transportation of the hydrogen fuel.[2] Herein, with the aid of transition state models, we decipher the mode of activity of the pincer-ligated manganese complex towards achieving the reversible hydrogenation and dehydrogenation process for the efficient H_2 storage and release.[3] We identified the critical contributions from the basic amino acids-specifically lysine and potassium lysinate-as well as the influence of solvent, counterions, and water in the reaction. In addition, we have probed into the role of non-covalent interactions during the capture and release of CO_2 with potassium lysinate, which enabled to achieve the carbon-neutral hydrogen battery system.[4]

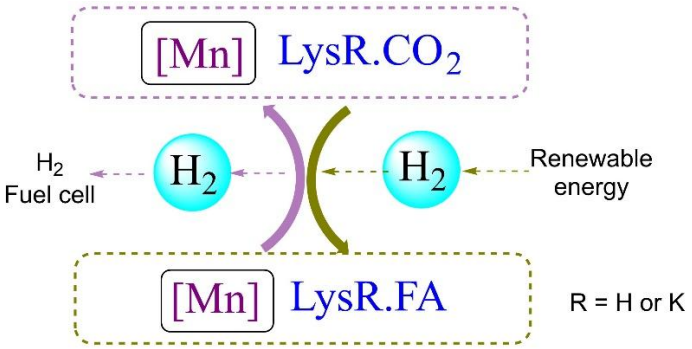


Figure 1 Reversible hydrogenation (of CO_2) and dehydrogenation (of formic acid) in presence of a manganese pincer complex with lysine (LysH)/potassium lysinate (LysK)

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Dynamics of Inhibition of Human Carbonic Anhydrases by Acetazolamide

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Acetazolamide (AZM) is a well-established competitive inhibitor of human carbonic anhydrases (HCAs), coordinating directly to the catalytic $Zn(II)$ ion in the active site [1]. Despite its widespread clinical use, AZM exhibits poor isoform selectivity, often leading to undesirable side effects. Moreover, recent in-cell NMR studies revealed a time-dependent dissociation of AZM-based drugs from intracellular $HCA\ II$ [2]. Motivated by these findings, we investigated the molecular mechanisms underlying AZM unbinding. Initially, QM/MM molecular dynamics (MD) simulations were employed to characterize the coordination environment of AZM at the $Zn(II)$ site, accounting for electronic effects, protonation dynamics, and reaction pathways associated with its detachment. Subsequently, classical MD simulations combined with enhanced sampling methods were used to explore alternative unbinding routes, transient binding events at surface pockets, and the final release of AZM into bulk solvent.

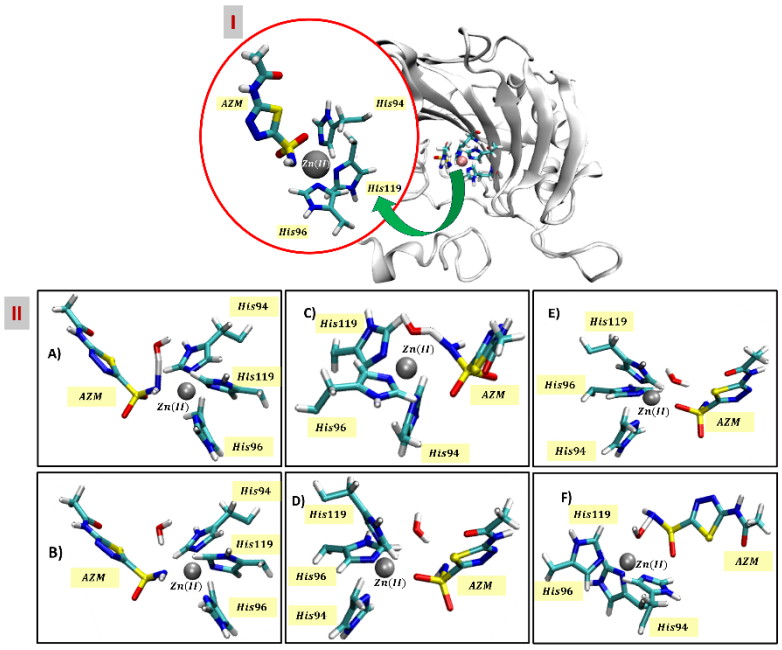


Figure1: (I)Structural snapshot of acetazolamide (AZM) binding to $Zn(II)$ at the catalytic core of HCA II. (II) Representative snapshots of change in coordination of $Zn(II)$ from QM/MM MD simulations incorporated with enhanced sampling.

References:

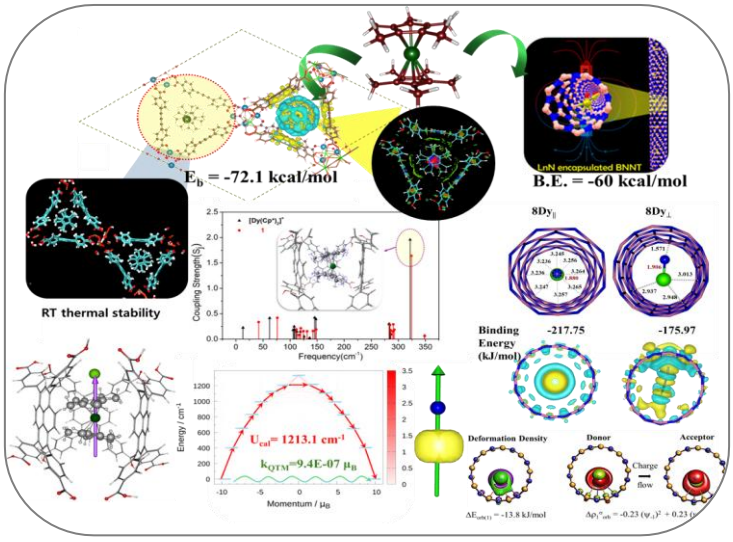
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Theoretical Chemistry Symposium
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Computational Modeling of Lanthanides-Based Single-Molecule Magnets Embedded in Nanostructured 1D, 2D, and 3D Frameworks

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Single-Molecule Magnets (SMMs)[1] offer promise for high-density data storage, spintronics, and quantum computing due to their ability to retain magnetization in the absence of an external field. Among these, lanthanide-based SMMs are particularly attractive owing to their large spin-orbit coupling, which enables large effective energy barriers (U_{eff}) and high blocking temperatures (T_B). However, integrating them into functional platforms is challenging, as surfaces or hosts can disrupt their magnetic behavior. Here, we present a systematic computational investigation combining periodic Density Functional Theory (pDFT) and multireference CASSCF calculations to explore the feasibility, dynamic stability, structure, bonding and magnetic properties of high-performance Dy-based SMMs in various hybrid architectures i) SMM@BNNT: Strongly axial Ln≡N (Ln = Dy, Tb) complexes, exhibiting record-high U_{eff} values (~2700 K), were modeled within boron nitride nanotubes (BNNTs) of varying diameters. The BNNT environment was found to stabilize the linear geometry of the complex while preserving its magnetic anisotropy ii) SMM@MOF: The $[Dy(Cp^*)_2]^+$ (U_{eff} ≈ 2200 K) is encapsulated within diamagnetic metal–organic frameworks (MOFs)—NU-1000, PCN-222-Zn, and MOF-177. The host–guest interactions and electronic structure were analyzed, revealing that the MOF cavities provide a protective environment for the magnetic core. The MOFs not only help provide long-range ordering of SMMs but also increase their stability by reducing the spin-phonon coupling. Electronic structure analyses using EDA, non-covalent interaction plots, AIMD, and projected density of states (pDOS) confirmed significant host-guest interactions across all platforms. CASSCF calculations indicated the preservation of strong axial magnetic anisotropy after encapsulation/surface adsorption. Our findings demonstrate that MOFs and BNNTs, can serve as viable platforms for hosting fragile SMMs, paving the way for their integration into next-generation molecular spintronic and quantum devices.



Schematic representation of SMM@1D, 3D nanostructures and their detailed analysis.

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Machine Learning-Based Fluorescence Prediction in the Chili RNA Aptamer System

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Fluorogenic RNA aptamers are short RNA sequences that activate the fluorescence of otherwise non-emissive small-molecule ligands, much like the green fluorescent protein (GFP) activates its intrinsic chromophore HBI.[1] These RNA-based tags can achieve high quantum yields and large fluorescence enhancements, making them powerful tools for live-cell imaging of RNA. One notable example is the Chili RNA aptamer, which binds HBI analogues and induces highly Stokes-shifted fluorescence across the visible spectrum.[2]

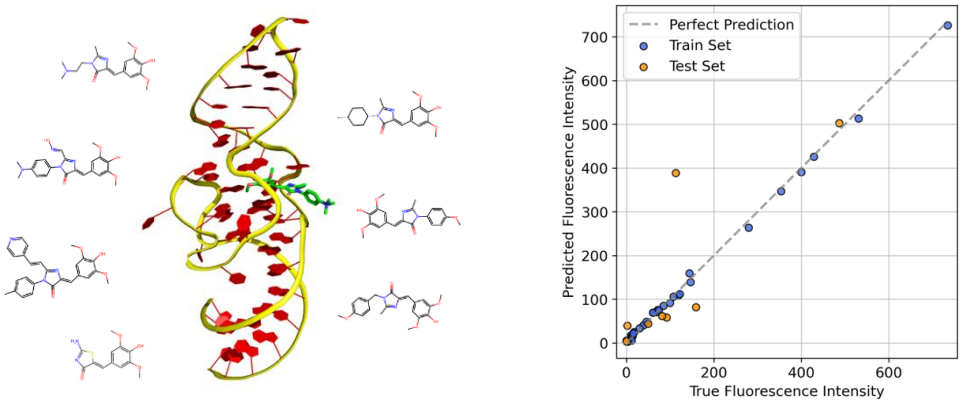


Figure 1 Left: Structure of the Chili RNA aptamer highlighting the ligand-binding pocket, with selected chromophores from the database. Right: Correlation between predicted and experimentally measured fluorescence intensities using the machine learning model.

Establishing clear correlations between ligand structure and photophysical performance remains a major challenge, often requiring computationally intensive approaches such as molecular dynamics simulations.[3] Therefore, we leverage an in-house database of HBI-derived chromophores and use supervised machine learning with quantum chemically derived descriptors to predict aptamer-induced fluorescence intensity directly from ligand structure. With this approach, we not only achieve highly accurate predictions but also uncover intrinsic structure–property relationships and identify new, highly promising ligand candidates.

References:

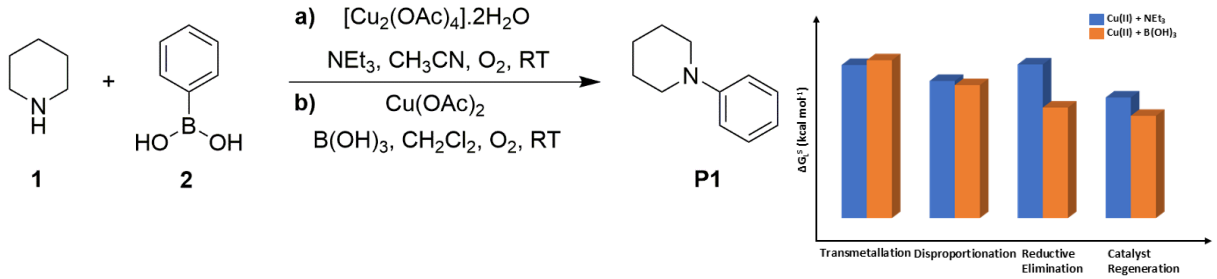
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Mechanistic Insights into Cu(II)-Catalyzed Chan-Lam Amination: A DFT-guided Base-Free, By-Product Promoted Approach

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C–N bond formation reactions have emerged as an essential element of synthetic chemistry, since they introduce nitrogen-based moieties into the organic framework, is especially in the fields of pharmaceutical and medical chemistry. A breakthrough comes with the utilization of oxidative cross-coupling employing Cu-catalysis, specifically the Chan-Lam (CL) cross-coupling method, which provides an economical, ligand-free, and mild reaction pathway.[1] The standard reaction conditions typically involve $Cu(OAc)_2$ catalyst in conjunction with NEt_3 as base (Scheme 1a).[2] The dissociation of the dinuclear Cu(II) paddlewheel complex in acetonitrile medium generates the active catalyst. Calculation reveals that the reaction initiates by $PhB(OH)_2$ coordination to the Cu(II) catalyst followed by transmetallation, disproportionation and finally reductive elimination. The product formation from the Cu(III) intermediate, generated via disproportionation, is reported to be the rate-determining step (δE = 26.0 kcal mol^{-1}).[3] Later, a simple approach was presented by Watson et.al., that involved inverting the conventional organoboron:amine stoichiometry and replacing the typical organic base (NEt_3) with transmetalation byproduct, boric acid, which was found to significantly improve the CL amination reaction.[2] Herein, we report the DFT-guided computational calculations to understand the detail mechanistic aspect of this Cu(II) catalyzed CL amination reaction following Watson's protocol, between an alkyl amine and phenyl boronic acid, under base-free condition employing $B(OH)_3$ as a promoter (Scheme 2b). Here the rate-determining step is clearly found to be transmetallation, unlike in the base-promoted reaction, where both transmetallation and the combined disproportionation and reductive elimination steps are competitive.[3,5]



Scheme 1: Reaction between piperidine (**1**) and phenyl boronic acid (**2**) using Cu(II) catalyst when a) NEt_3 is used as a base b) reaction is promoted by $B(OH)_3$

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Generative AI Mediated Anti-Microbial Peptide Design

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Anti-Microbial Resistance (AMR), recognized as one of the most critical global health crises, poses a significant challenge. With the discovery of new antibiotics slowing down, the need has arisen for the discovery of noble Anti-Microbial Peptides (AMP). These are a class of peptide with length ranging between 10 to 50 and are naturally produced by many organisms[1]. The main advantage of AMPs over antibiotics come from its mechanism of action. But the discovery of AMPs is limited by the vastness of the sequence space as for a 32 residue peptide it can cover approximately 4.5×10^{41} peptides[2]. So, to tackle this limitation as well as introducing diveristy in the sequene space, in this work we propose a decoder only transformer model for generation of novel AMPs[3]. For this purpose a decoder only transformer model was pre-trained on peptide data from Uniprot to learn the underlying grammar of peptides. Then we trained a AMP classifier using the embeddings from the first transformation layer of the model. Then we performed supervised fine-tuning of the model where we also introduced the conditions for the type of AMP generation as well as we injected the structure and property information for structure aware generation. At last we validated the model generated AMPs with some peptide physicochemical property, toxicity measurement and molecular dynamics simulation.

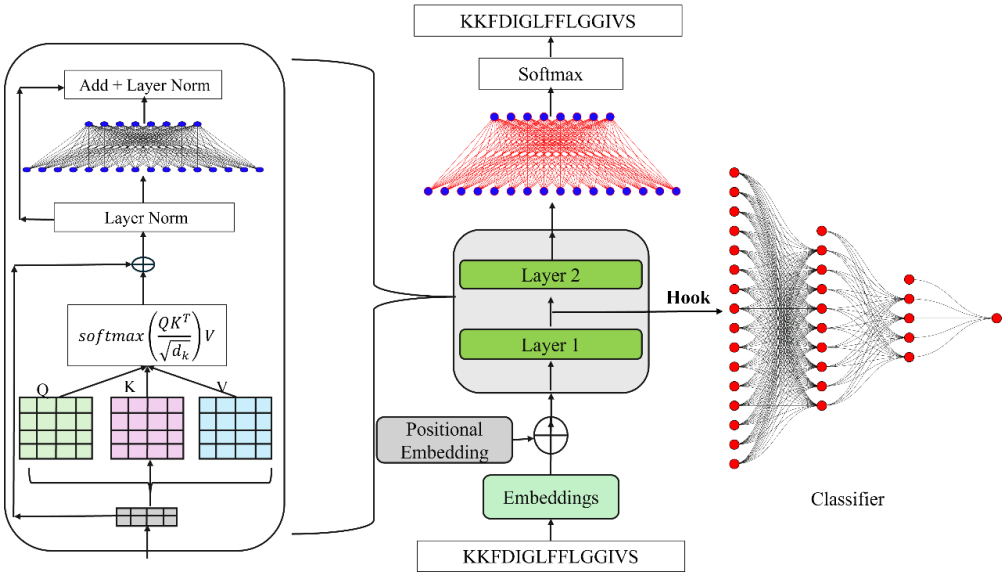


Figure 1: The architecture of the decoder only transformer model for AMP generation along with the classifier model which takes embeddings from the first layer as input.

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Studies of amine bond Surfactants using Molecular Dynamics Simulations.

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Surfactants, due to their amphiphilic nature, find extensive use in industries such as printing, detergents, cosmetics, food, pharmaceuticals, oil recovery, and nanomaterial synthesis.[1] Among them, amine bond-based cationic surfactants have gained attention for their strong surface activity, antibacterial properties, and rapid degradability compared to traditional types.[2] Computational techniques, particularly molecular dynamics (MD) simulations, provide molecular-level insights into surfactant aggregation and complement experimental findings in designing surfactants with tailored applications.[3]

In this work, MD simulations were performed to investigate the aggregation behaviour of oligomeric amine bond surfactants (Fig.1) in aqueous solutions and at the liquid-vapor interface. The model systems include monomeric, dimeric, and trimeric surfactants, where increasing the number of linked monomeric units leads to a decrease in aggregation number and significant changes in aggregate morphology. Monomeric surfactants primarily form spherical micelles, while dimeric and trimeric surfactants assemble into elongated, worm-like structures (Fig.2). Additionally, stable π–π stacking interactions between benzene rings were observed, which contribute to aggregate stability. These results align with experimental observations and highlight the potential of oligomeric amine bond surfactants for advanced applications.

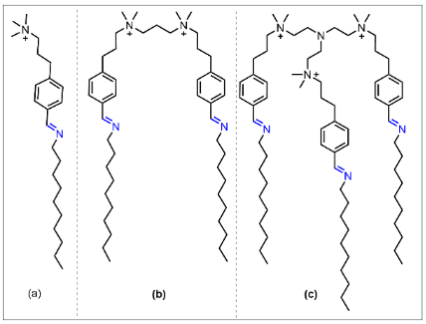


Figure 1 (a) SIS, (b) GIS, (c) TIS.

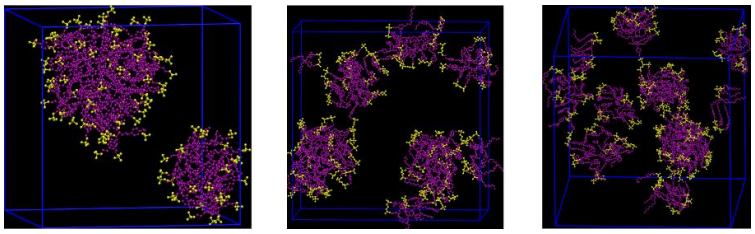


Figure 2 Snapshot of aggregates.

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Unveiling Electric Field Catalysis in Lewis Acid-Mediated Ring-Closing Carbonyl–Olefin Metathesis and Oxa Diels–Alder Reactions

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Electric field (EF) catalysis has emerged as a versatile approach for precisely controlling chemical reactivity and selectivity, which has been explained by theory and demonstrated by experiments. This DFT study explores how Lewis acids create internal electric fields that enhance ring-closing carbonyl–olefin metathesis (RCCOM) and examines the impact of external electric fields on electron transfer in LA-catalyzed Oxa Diels–Alder (ODA) reactions between cyclopentadiene and formaldehyde.

In RCCOM, Lewis acids create strong electric fields aligned with the reaction path that help to mix ionic and covalent character. This realigns electron orbitals, enabling a smoother, ionic-like pathway during key steps like cycloaddition and carbonyl–ene reactions.[1] The internal EF works together with traditional Lewis acid effects to boost catalysis.

In the ODA reaction, external EFs speed up the reaction in one direction while slowing it in the opposite. The inhibition reaches maximum at the electrostatic resistance point (ERP).[2,3] Strong inhibitory EFs can override the usual Lewis acid catalysis and switch over to Lewis base catalysis through a different electron demand pathway.[4] This makes the EF a useful tool to adjust reactivity,[5] switch between Lewis acid and base roles, and a probe to explore electron transfer behavior in complex mechanisms.

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Exploring Porphyrin based 2D c-MOF as Single Atom Catalyst for Carbon dioxide Reduction Reaction

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With the rise in global energy demands, the carbon dioxide emission rate is increasing alarmingly which is the major contributor to global warming. Capturing and converting this CO_2 into useful chemicals can potentially help to mitigate CO_2 levels[1]. Electrochemical reduction of CO_2 is an efficient way to convert CO_2 into useful chemicals. However, CO_2 being a stable and unreactive molecule, developing catalysts for efficient CO_2 reduction reaction (CO2RR) with desired selectivity is a need of the hour.

In this work, an experimentally reported porphyrine based 2D conducting metal organic framework (2D c-MOF) doped with Co atom is considered to explore its activity towards CO2RR.[2] Two reaction pathways[3] for CO2RR to different end products based on possible CO_2 adsorption via C and O atoms are being examined using DFT studies. Free energy changes associated with all the elementary reactions are calculated to obtain the fee energy profile for overall CO2RR as shown in Figure 1.

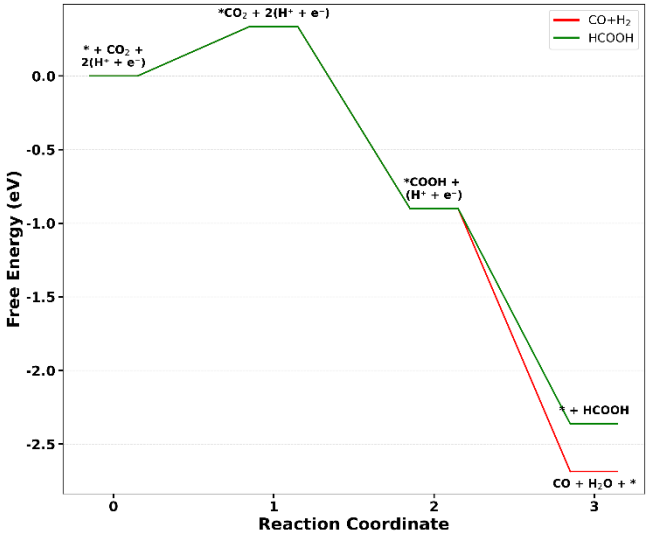


Figure 1: Free Energy Diagram for CO and HCOOH production

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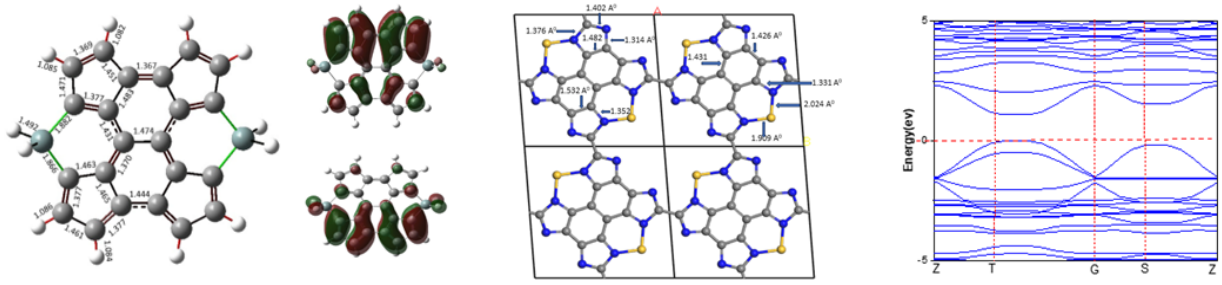
Two Wrongs Make a Right :A Edge sharing Indacene Dimer

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The monomer of *as*-indacene is known to be antiaromatic and reactive due to its 4n-π electrons, while its dianion and dication are aromatic with distinct distortions. When two AS indacene units are edge-shared through the bare benzene edge with SiH_2 linkers to keep planarity(Figure 1a), it undergoes a zwitterionic state just like Azulene[1], where five and seven-membered fused rings exhibit a charge separation of (-1) and (+1). Biindacene core have charge separation (-2) charge on one side and (+2) charge on the other side, reducing its symmetry to C_{2v}. The dimer A singlet (C_{2v}) is more stable than the triplet state by 0.63 kcal/mol at the standard B3LYP/6-31G(d) level of theory. It has a narrow HOMO-LUMO gap of 1.56 eV where HOMO and LUMO are concentrated on the opposite sides of the molecule. It also exhibits a significant dipole moment of 1.53 D, resulting from pronounced intramolecular charge separation. The wave function is found to be stable for both the singlet and triplet states. An extended 2D lattice constructed with this building block shows a narrow band-gap of 1.093eV. These unique electronic configurations, combined with an extended, polarized π-framework suggest exceptional optoelectronic properties and potential for anti-kasha fluorescence. The near degeneracy of orbitals/bands and the strong electron-phonon coupling arising from the uniqueness of the geometry may lead to strong dynamic Jahn-teller/vibronic mixing. The fast vibronic fluctuations are a phenomenon that is believed to aid superconductivity and colossal magnetoresistance. The molecule's inherent polarity and small energy gap make it a prime candidate for application in organic photovoltaics as a charge transport material, in light-emitting diodes, polarizable sensors and as a functional component in next-generation optoelectronic devices.



(a) (b) (c) (d)

Figure 1. (a) Structure of Biindacene with SiH2 linkers (using B3LYP). (b) HOMO of Biindacene with SiH_2 linker and LUMO of Biindacene with SiH_2 (c) Extended structure (d) it's band structure

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A Computational Investigation of the Photochemical Transformation of 1,3-Cycloheptadiene to Bicyclo[3.2.0]Heptene

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Conical intersections (CIs)[1] are central to ultrafast nonadiabatic relaxation and decisively govern photochemical selectivity. The electrocyclic ring-closure reaction of 1,3-cycloheptadiene conformers with Cs and C_2 symmetries to bicyclo[3.2.0]heptene is investigated.[2] For that, the Cs and C_2 conformers with their probable Cs-product and C_2-product are located as optimized geometries. The transition states (TSs) and the S_1/S_2 and S_1/S_0 CIs optimization were performed. A disrotatory TS is identified for the Cs-reactant to Cs-product pathway, while two conrotatory TS are observed, one connects the Cs-product to a cis,trans-cyclohepta-1,3-diene intermediate, and another connects the C_2-product with the C_2-reactant. Reaction coordinate interpolation reveals that only the Cs-product channel is viable, as the C_2-product route presents a high-energy, prohibitive barrier. Nonadiabatic surface hopping simulations from the S_1 state yield exclusive formation of the Cs photoproduct with quantum yields of ~7% and ~2% from Cs and C_2 conformers, respectively, due to differences in $S_1 \rightarrow S_0$ decay dynamics at the CI of S_1/S_0 seam. These results establish the mechanistic primacy of conical intersections in dictating product distribution in electrocyclic photoreactions[3] and provide insights relevant to photomedicine,[4,5] nanotechnology,[6,7] etc.

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Efficient targeting of interior excited states using inexact Lanczos methods and tree tensor network states

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Accurate determination of interior excited states is crucial for elucidating a range of phenomena, including core ionization[1], conical intersections[2], and high-frequency regions of vibrational spectra[3–5]. However, compared to many efficient eigensolvers for ground and low-lying excited states, there are much fewer effective algorithms available for interior states. Here, we present an efficient eigensolver tailored for interior vibrational states using the tree tensor network state (TTNS) ansatz[5–6], employing an inexact Lanczos method[7–8]. The method is first benchmarked by application to five distinct energy levels. Subsequently, we formulate an approach to compute all eigenstates within a specified energy window. Using this strategy, 122 states from two different spectral regions of the 12-dimensional acetonitrile molecule are accurately calculated. The algorithm also supports *state following*, demonstrated by targeting a Fermi resonance state of the Zundel ion. Finally, selected excited states of the higher-dimensional (33D) and more fluxional Eigen ion are computed, enabling the first full-dimensional simulation of its excited states.

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Dopant and nucleophile directed catalytic selectivity of Graphene Oxide for cyclic and polycarbonate formation - A DFT study

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The cycloaddition of epoxides with CO_2 is a sustainable route to cyclic and polycarbonates, yet product selectivity remains a key challenge.[1] In this work, the DFT methods were employed to study pristine graphene oxide (**GO-27**) and its doped analogues, nitrogen-doped GO (**NGO**)[2] and boron-doped GO (**BGO**).[3] The **GO-27** stabilises the substrates through hydrogen bonding at the -OH and -COOH edges, with the -COOH edge being kinetically favoured by +5.5 kcal/mol. However, **GO-27** shows poor product selectivity, as the barriers for the cyclic carbonate (+14.2 kcal/mol) and polycarbonate (+12.2 kcal/mol) are comparable. Electronic tuning achieved by doping improves the selectivity. **NGO** enhances the electron donation nature, stabilises the ring-closure step and favours cyclic carbonate (10.2 kcal/mol) over polycarbonate (+14.1 kcal/mol). In contrast, **BGO** enhances the electron-accepting nature, promotes chain initiation, and shifts the selectivity towards polycarbonate formation (+4.5 kcal/mol) over cyclic carbonate (+10.2 kcal/mol). Further, the nucleophile effects also play a crucial role in tuning the product selectivity. The poor leaving groups like CN^- and N_3^- hinder the formation of cyclic carbonate and strongly favour the formation of polycarbonate by +37.8 kcal/mol and +13.3 kcal/mol, respectively. Therefore, this work demonstrates that the graphene oxide can be systematically tuned through electronic effects or nucleophile choice to achieve targeted product selectivity in the cycloaddition reaction between epoxide and CO_2.

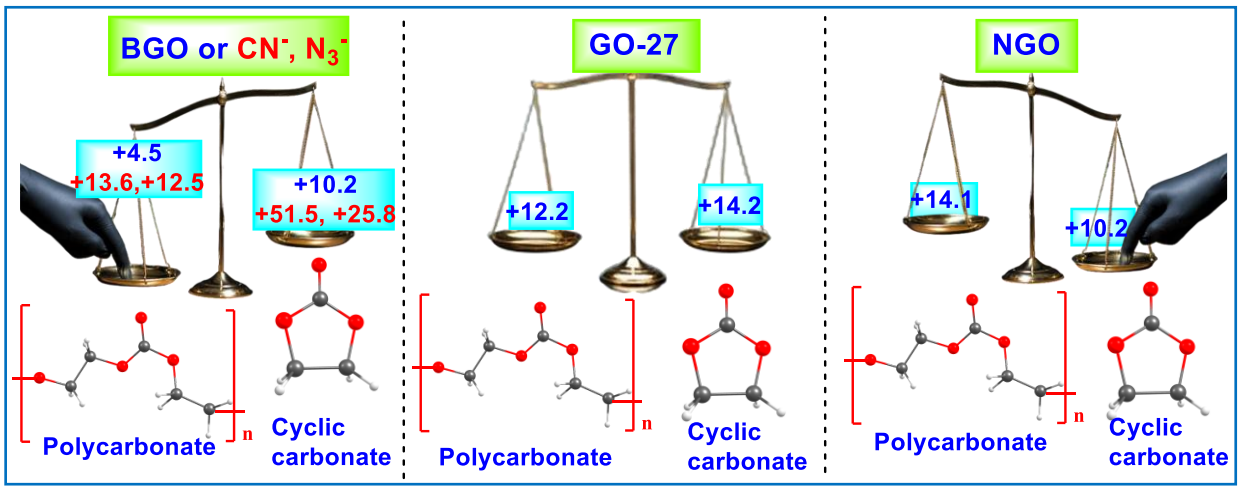


Figure 1. Schematic representation of **GO-27**, **NGO**, and **BGO** exhibiting product selectivity between the cyclic and polycarbonate, wherein the numbers indicate the activation energy required in kcal/mol.

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Unveiling the Role of Ion Pairs in Determining Electrolyte Stability and Solid Electrolyte Interphase Formation in Lithium Metal Batteries

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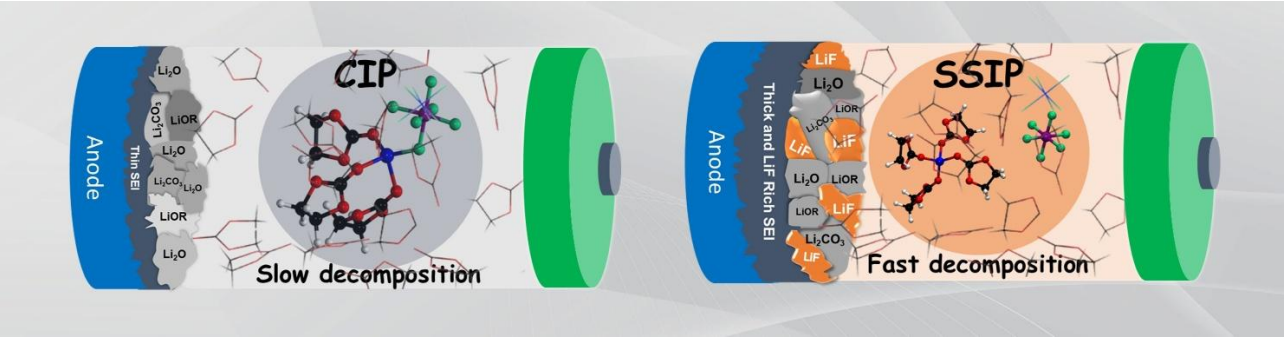
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Lithium metal batteries (LMBs) are crucial to the electronics industry, providing power to most common devices used daily.[1] Despite extensive global research, current LMBs still fall short of meeting global energy targets. As a result, improving LMBs energy density, power density, and cycle life remains a key research focus, particularly in advancing cathodes, anodes, and electrolytes. Interface engineering, especially at the electrode-electrolyte interface (called solid electrolyte interface (SEI) at anodes), has emerged as a promising strategy to enhance LMBs performance, particularly with Li-metal anodes.[2,3] The electrode-electrolyte interface (EEI) formed by the decomposition of electrolytes on the electrode surface was found to have a crucial role in determining the performance of Li metal batteries (LMBs).[4] The EEI formation kinetics and structure depend on the structure of the electrolyte and has a critical role in determining its reactivity towards the electrodes and thus the EEI formation mechanism and kinetics. We noted that there are disparities over the structure of some of the commonly used electrolytes in LMBs, especially on the solvation structure, in literature.

Despite many studies over the years, the mechanism, kinetics, and factors influencing the SEI formation remain elusive. In this regard, we employed ab initio molecular dynamics (AIMD) simulations to analyze the role of electrolyte structure in determining the mechanism and kinetics of SEI formation. Specifically, we investigated the effect of two types of ion pair (IP) configurations that our simulations revealed to be present and playing a significant role in determining the electrolyte structure: contact IPs and solvent-separated IPs. AIMD simulations provide fundamental insights into the mechanisms and kinetics of SEI formation, reveal structure-reactivity relationships that govern electrolyte decomposition on the Li metal surface, and propose strategies to enhance electrolyte stability and tailor the composition of SEI.



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Design of Workflows for Accelerated Solvent Screening for CO_2 Capture: A Hybrid DFT-AI/ML Approach

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The design of efficient solvents is critical for addressing climate change by enabling effective gas separation in industries (e.g., CO_2 capture and utilization) like power generation, natural gas processing, and wastewater treatment. Solvents are also vital in pharmaceutical synthesis and energy storage. The most commonly solvents for CO_2 capture include amines and their blends (phase-separating solvents), deep eutectic solvents and ionic liquids[1]. Traditional solvent screening methods which rely heavily on experiments are not just slow but also expensive, necessitating advanced computational approaches. The current study integrates the first principles density functional theory (DFT) and Artificial Intelligence (AI) with the experimental data to accelerate the design of novel solvents for efficient CO_2 capture and utilization. The integration of AI is revolutionizing solvent discovery by combining quantum chemical (DFT) descriptors, molecular properties (via. solvation and transfer free energies, Log S, and Log P), and empirical data into predictive frameworks. A variety of classical ML algorithms, along with deep learning approaches, are used to accurately predict solvent-CO_2 interaction energies and thermodynamic parameters[2]. Machine learning models further analyze large chemical datasets to identify top performing candidates, while generative AI explores novel molecular compositions optimized for selectivity and lower regeneration energy[3]. These data-driven approaches also reveal key molecular factors influencing CO_2 affinity, enabling more rational and targeted solvent design. The hybrid DFT–AI/ML pipeline supports high-throughput virtual screening, evaluating thousands of solvent candidates in months rather than years. We explored solvation databases, including MNSol-2012[4], AqSolDB[5], and Combisolv(QM and EXP)[6], to which yielded extensive datasets of solvation and hydration free energies, and Log S values derived either from empirical methods or computational studies. These datasets are being curated to extract key insights for developing a novel pipeline (which employs a combination of structure based screening, DFT level analysis and use of advanced AI/ML tools like NLPs and transformers) that accelerates solvent design purely based on physicochemical properties and geometric features. By reducing reliance solely on empirical testing, this strategy minimizes costs and material waste, providing a scalable, sustainable, and intelligent framework for solvent innovation in CO_2 capture, catalysis, green chemistry, and materials science.

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Impact of Electron Attachment on Dipeptides Conformers

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In this investigation, we study the impact of electron attachment on the conformers of the dipeptides Alanyl Glycine and Glycyl Alanine. The low-lying conformers of the dipeptides are identified from the dihedral angle scan, followed by atom-centered density matrix propagation (ADMP)[1,2] simulations to examine the impact of electron attachment at 2.0 eV. The singly occupied molecular orbitals (SOMOs) revealed that a transition from a dipole-bound state to a π∗ valence-bound state occurs for the conformers. The results showed that different conformers exhibit distinct impact on electron attachment, and strong intramolecular hydrogen bonds enhance stability towards dissociative electron attachment (DEA). In the latter part of the work, two low-lying π∗ resonance states associated with the DEA process (involving a π∗ → σ∗ transition) were characterised using the complex absorbing potential (CAP) method[3,4]. The calculated results found good agreement with experimental results for Alanyl Glycine and Glycyl Alanine in the gas phase.

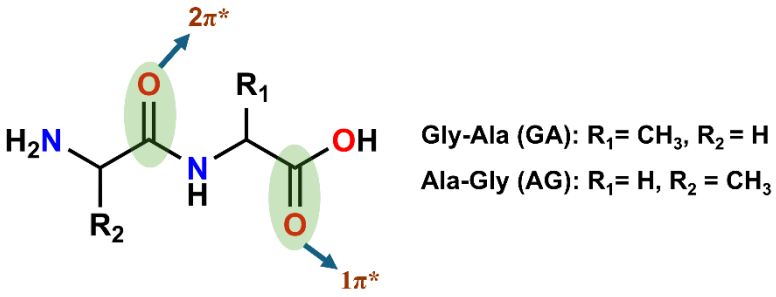


Figure 1 Schematic representations of the dipeptides Gly–Ala and Ala–Gly, and two possible π∗ electronic states

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Aza-Triphenylene-Based Covalent Organic Framework: Anode for High-Efficiency Sodium-Ion Batteries

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This study explores the potential of a newly developed aza-triphenylene-based covalent organic framework (aza-COF) as an anode material for sodium-ion batteries (SIBs), utilizing density functional theory calculations [1,2]. The findings reveal that the two-dimensional aza-COF behaves as a direct band gap semiconductor with a band gap of 1.02 eV. Upon sodium insertion at the most favorable site, the material undergoes a transition from semiconducting to metallic behavior, enhancing its electrical conductivity. The aza-COF exhibits a sodium-ion diffusion barrier of 0.78 eV, a high theoretical specific capacity of 602.3 $mAhg^{-1}$, an energy density of 1259.5 $mWhg^{-1}$, and an average operating voltage of 0.62 V, well within the optimal range of 0.1–1.0 V as shown in Fig 1. Its structural flexibility further supports its effectiveness in battery applications. Moreover, aza-COF shows strong interaction with electrolytes, reinforcing its promise as a highly effective electrode material. These compelling theoretical results indicate that aza-COF could function as a highly efficient anode material for SIBs.

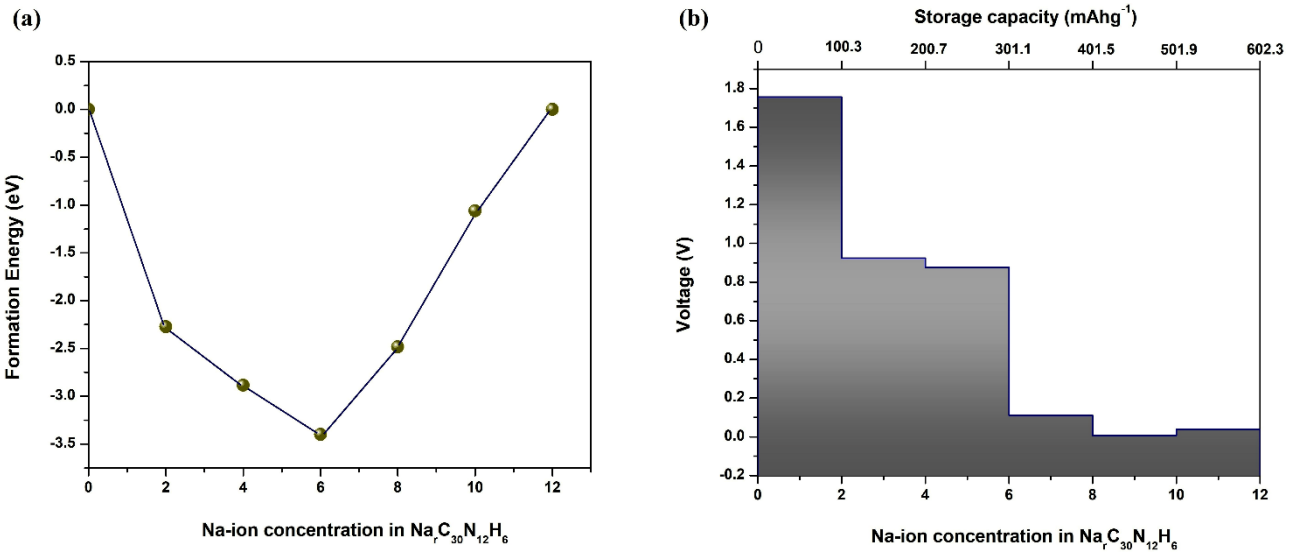


Fig.1 (a) A convex hull diagram representing the changes in formation energy across varying sodium ion concentrations, along with (b) the associated voltage curve corresponding to the convex hull for different levels of Na-ion content.

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Molecular Engineering on Pechmann Dyes for Singlet Fission

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Singlet fission (SF), a process in which two triplet excitons are produced from a singlet exciton in organic chromophores, offers a promising strategy to overcome the efficiency constraints of the Shockley–Queisser limit in photovoltaic devices. In this study, the Pechmann moiety, represented by (E)-3,3′-bifuranylidene-2,2′-dione heterocyclic systems, is examined to explore its singlet fission characteristics. This family of organic chromophores, with cross-conjugated lactone rings, shows a unique ability to exhibit singlet fission across various substitutions in different carbon atoms, distinguishing it from other molecules. The feasibility of singlet fission is examined using excited-state energy calculations, analysis of diradical and tetraradical character, and frontier molecular orbital studies. The role of electron-withdrawing and electron-donating substituents at radical centers is also analyzed to understand their influence on the singlet–triplet energy gaps and compliance with the energy criteria $E(S_1) \geq 2E(T_1)$ and $E(T_2) \geq 2E(T_1)$. The results highlight the lesser-known potential of the Pechmann moiety as a promising singlet fission candidate, and propose design strategies for developing Pechmann dyes with enhanced efficiency

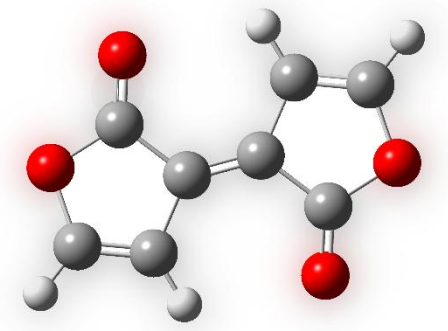


Figure 1: The Pechmann lactone moiety

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Cation-π Interactions Involving Graphynes: An Intermolecular Force Field Formulation Featuring Ion-Induced Dipole Effects

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Over the past few years, graphynes (GYs), one of the latest family of carbon allotropes, have been investigated as promising materials for various applications, including alkali ion batteries.[1, 2] Developing analytic approaches for describing potential energy surfaces for the binding and transport of alkali ions to the carbonaceous electrode materials is imperative for large-scale simulations, and is necessitated by the high computational demands of *ab initio* methods for such systems. In this study, we developed effective analytic models to accurately capture cation-π interactions between alkali metal ions (Li^+, Na^+, K^+) and GYs, which are crucial for ion storage and transport within nanoporous GY frameworks. Prior literature reports on developing improved force fields for cation-π interactions have predominantly focused on small aromatic molecules.[3] Here, we report that the commonly used 12-6 Lennard-Jones (LJ) potential combined with electrostatics (EL) is insufficient for capturing cation-π interactions, as it fails to account for the ion-induced dipole effects that are crucial for the problem at hand.[4, 5] To address this, we implemented the 12-4 LJ potential + EL and the improved Lennard-Jones (ILJ) potential[6] + EL formulations that accurately incorporate the short-range repulsions and long-range attractions. We developed and validated parameter sets based on interaction energy curves from density functional theory, enabling a reasonably accurate modeling of cation permeation and surface dynamics of cations on GYs.[5] This work advances the understanding of cation-π interactions in GYs and introduces computationally efficient models that can be adopted for large-scale simulations.

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Competition between Electron-Transfer Mediated Decay and proton transfer process in $Li^+(H_2O)_n$ (n=1,2) Complexes

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This study investigates the Electron-Transfer Mediated Decay (ETMD) process in micro-solvated lithium ions, $Li^+(H_2O)_n$. We generated potential energy curves (PECs) and calculated ETMD decay rates using IP-EOMCCSD for the first solvation shell (Li^+-OH_2) by varying the Li-O distance and O-H bond length to quantify the effects of solvation geometry and water polarization on the decay dynamics. Furthermore, we explored the role of proton transfer in the second solvation shell ($Li^+(H_2O)_2$) by generating PECs and decay rates along the proton transfer coordinate. Our results demonstrate that both the solvation structure and proton dynamics significantly modulate the ETMD rate, revealing a strong coupling between nuclear motion and electronic decay processes. We also demonstrate the comparative analysis with H_2S as a neighbor highlights the role of the neighboring electronic & molecular properties. From BOMD dynamics it is establish that ETMD is not a static process but is profoundly enhanced by specific nuclear rearrangements, particularly proton transfer, offering new avenues for controlling radiation less non-local decay in different environments.

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An Approach Based on Conceptual Density Functional Theory to Predict the Quenching Rate of Excited Carbazoles Donors in Bimolecular Electron Transfer Reactions

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Abstract

The current study investigates the qualitative trend of the rate of bimolecular electron transfer reactions from excited-state carbazole derivatives to acceptors, i.e., (i) organic acids, (ii) acetates, and (iii) halocarbons in a low-polarity solvent, tetrahydrofuran (THF).[1] The conceptual density functional theory (CDFT) based comprehensive decomposition analysis of stabilization energy (or CDASE) scheme is used to calculate the values of reaction-free energy.[2] The observed trend in the CDASE scheme-based stabilization energy suggests that it can be used qualitatively as a substitute for experimentally obtained reaction-free energy. The classical Marcus model [3] is used to evaluate the reorganization energy values. An attempt is made to establish the correlation between the sum of reorganization and stabilization energy with the bimolecular quenching rate constant of electron transfer reactions in the spirit of Marcus theory.[4] As these three types of electron transfer reactions follow diffusive conditions, only the solvent reorganization energy is more sensitive and assumed to play a predominant role. It is observed that as the sum of the CDFT-based stabilization energy and the reorganization energy values decreases, the experimental quenching rate constant for the chosen weakly coupled donor-acceptor systems increases.[5] Thus, the generated data aligns very well with the traditional Marcus theory of electron transfer.

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Bonding Insights into Metavalent Materials for Next-generation Memory

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Phase change materials have gained a lot of attention because of their use in phase change memory (PCM) technology. This technology can overcome the von Neumann bottleneck through in-memory computing. It is especially valuable in artificial intelligence applications that need fast data transfer. Consequently, figuring out the bonding mechanism in these materials is vital for creating better PCM materials. Recently, a new bonding mechanism called metavalency was introduced to explain the bonding in phase change materials. Metavalent materials have a bond order close to half, a large Born Effective Charge (BEC), a low band gap, moderate electrical conductivity, and a large optical dielectric constant. However, their bonding characteristics are very similar to those of well-known hypervalent and partially σ-bonded systems, raising important questions about whether metavalency is genuinely a different bonding mechanism. In this study, we use molecular orbital theory and DFT calculations to demonstrate that the known metavalent compounds are electron-sufficient or rich hypercoordinate systems with partial σ bonds primarily formed by p-p overlap. These compounds show low ionicity, a low band gap, and a large BEC. We suggest that electron-sufficient/rich hypercoordinate systems with nearly half bond order can be classified as metavalent. This means they belong to a distinct group of compounds, even though the bonding mechanism is not new. If these compounds have low ionicity, a low band gap, and an extended lattice, they could be promising candidates for PCM applications. This improved understanding of metavalent bonding offers a solid foundation for the thoughtful design of new PCMs, leading to progress in phase-change memory technology.

Theoretical Chemistry Symposium
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Monitoring Solution Structure of Polynucleotides using Spectroscopy of Raman Optical Activity

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Understanding the solution-phase structures of nucleic acids is essential for elucidating their function and reactivity. Raman optical activity (ROA) spectroscopy, which measures differential scattering of right and left circularly polarized light, offers high sensitivity to molecular conformation and stereochemistry. However, its application to nucleic acids has been limited due to the structural complexity and challenges associated with spectral interpretation.[1, 2]

In this study, we combine experimental Raman and ROA spectroscopy with advanced computational modeling to investigate structure-spectra relationships in the polynucleotides. Spectral simulations are performed using molecular dynamics (MD) simulations and density functional theory (DFT) calculations, with the aid of the fragment-based Cartesian Coordinate Tensor Transfer (CCT) approach,[3] which enables efficient treatment of large nucleic acid systems. Our results demonstrate that the ROA spectra reliably reflect conformational features and temperature-induced structural changes. Furthermore, experimental spectral intensities can serve as effective benchmarks for evaluating and refining MD force fields.

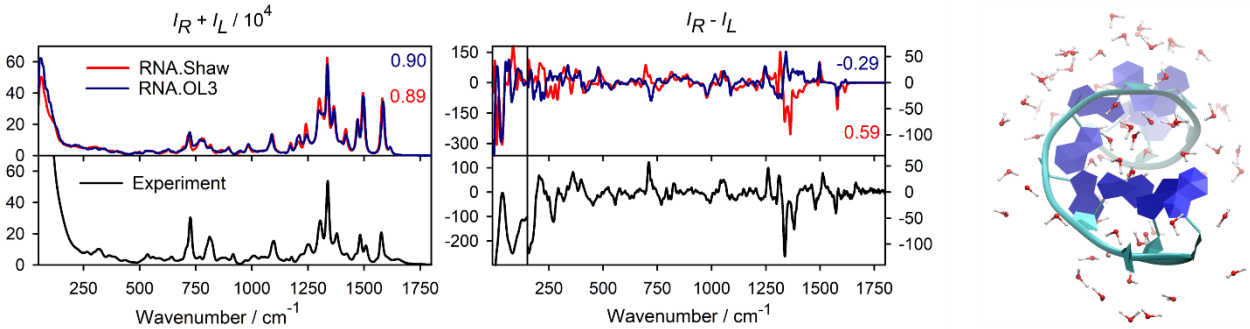


Figure 1. Experimental Raman and ROA spectra of polyA compared with calculations based on the RNA.OL3 and RNA.Shaw force fields.

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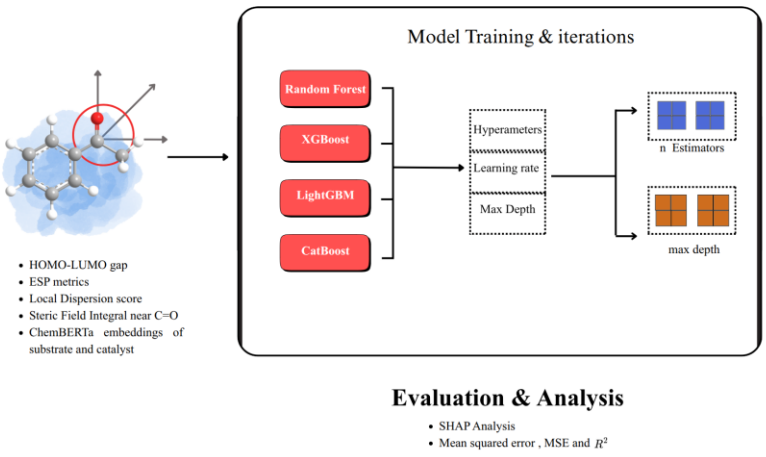
Theoretical Chemistry Symposium
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Machine Learning Based Model Predict Enantiomeric Excess in Carbonyl Reductions Using Hybrid Structure and Context Features

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We predict the enantiomeric excess of carbonyl reductions using a hybrid featurization that encodes the substrate and the catalyst. We opt for SMILES with ChemBERTa and we concatenate these learned embeddings with quantum based descriptors such as the HOMO to LUMO gap, electrostatic potential metrics, and a local dispersion score. We add steric descriptors such as Sterimol and a steric field integral near the carbonyl. We also include reaction context variables so additives and solvents are seen by the model alongside structure.We then train a suite of classical regressors to predict the enantiomeric excess . The base learners cover Random Forest, XGBoost, LightGBM, and CatBoost, and we also build a stacked ensemble with a Ridge meta learner that combines out of fold predictions from the base models. We sweep the number of trees in the Random Forest and select the best setting by cross validated error. The pipeline computes mean squared error and R^2 on validation and test and reports the mean and the standard deviation across seeds and folds. When synthetic augmentation is used, the synthetic samples are kept grouped with their parent reactions inside a single fold to avoid leakage. We also probe feature importance with SHAP style attributions so that steric, electrostatic, and dispersion terms can be linked back to chemical intuition and to guide condition selection.



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1. Machine Learning Based Model Predict Enantiomeric Excess in Carbonyl Reduction Reactions
J. Kaur, P. P. Singh, M. Jakhar, C. Dey, K. Thakran, R. Mayank, Shihan V C, S. Chakraborty* (Submitted)

Unraveling the Reaction Mechanisms and Kinetic Pathways of OH-Initiated Oxidation of Allylcyanide: Insights into Atmospheric Chemistry

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A detailed investigation into molecular-level insights of the reaction mechanisms, kinetics, atmospheric lifetime, global warming potential and secondary degradation processes of allyl cyanide (CH_2=$CHCH_2CN$) is imperative because of its broad industrial applications. In this regard, we have performed a density functional theory (DFT) study of the CH_2=$CHCH_2CN$ molecule initiated by OH radical using M06-2X functional combined with 6-311++ G(d, p) basis set. Furthermore, all species underwent energetic refinement using the high-accuracy CCSD(T)-FC method while maintaining the same basis set. We have explored the potential energy surface (PES) of the H-abstraction reactions by OH radical as well as OH-addition to the unsaturated C-atoms of the CH_2=$CHCH_2CN$ molecule. The PES analysis and thermochemical calculations demonstrate that the OH-addition channels contribute more significantly to the overall reaction mechanism compared to H-abstraction pathways. The rate constants of all the reaction channels are determined using canonical variational transition state theory (CVTST) throughout the temperature range of 250-500 K. The cumulative rate constant of the titled reaction was observed to be 2.42×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298 K. The lifetime of the CH_2=$CHCH_2CN$ molecule is very short due to the reaction with OH radical and it is estimated to be 23 days and 3 weeks. The values of Global warming potentials (GWPs) for the titled compound are estimated to be 0.019, 0.005 and 0.001 in 20 years, 100 years and 500 years' intervals, respectively.

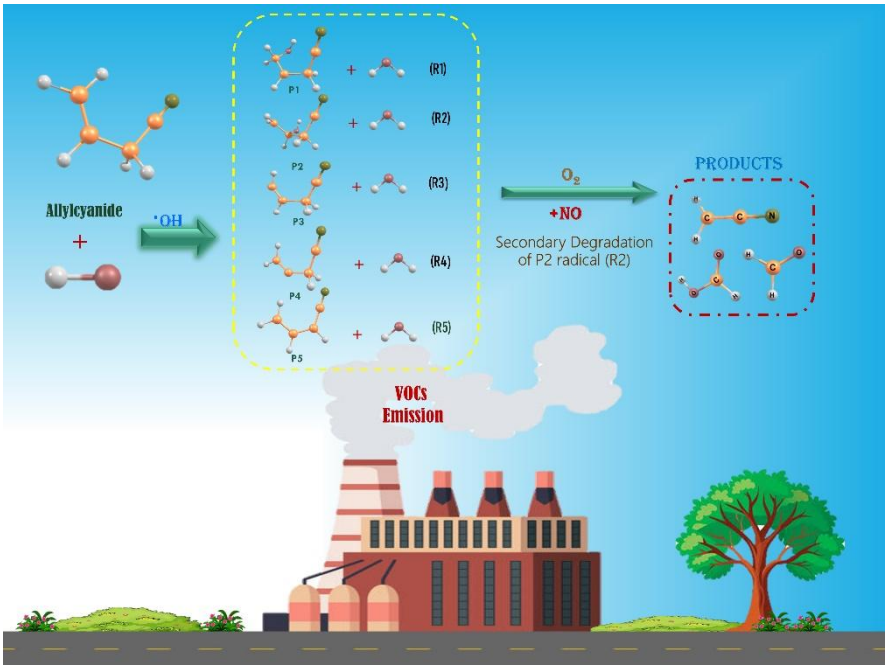


Figure 1 OH-Initiated atmospheric oxidation of allylcyanide.

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Theoretical Chemistry Symposium
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Identification of Methylated DNA Biomarkers by Nanosensors Based on Hydrogenated Borophene

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Identification of methylated DNA using 2D hydrogenated borophene, Rect-$1H_{top}$, Rect-$1H_{bridge}$, and Rect-$2H_{top}$ has not been studied. In this work, we report the adsorption of 5-methylcytosine and 5-hydroxymethylcytosine using the DFT and AIMD simulations. The 5-methylcytosine and 5-hydroxymethylcytosine are expected to fluctuate when they come closer to the surface of hydrogenated borophene. To address this, we focus on the adsorption type in different binding sites and orientations. The binding energies were found to be higher in the horizontal orientations. Our calculated density of states after the adsorption of the molecules shows the mixing of orbitals overlaps around the Fermi level (E_F), indicating that the metallic property is preserved. The Charge density difference (CDD) has been performed to visualise the distribution of charge between the hydrogenated borophene and the methylated DNA, and the direction of flowing charge is calculated using the plane-average charge density difference, indicating the charge gain from the methylated DNA. Furthermore, the transmission function T(E) is calculated using a non-equilibrium Green's function, and it is found that Rect-$2H_{top}$ has the highest electronic transport. Moreover, the current voltage (I-V) characteristics are calculated, ranging from 0 to 1 V, to generate an electrical current that serves as a signal for detecting different methylated DNA [1,2].

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Mechanistic Pathways of Crown Ether–Stabilized Alkali Metal Phosphides in Alkyne Hydrophosphination: A DFT Study

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Hydrophosphination (HP) is an atom-economical and sustainable strategy for constructing P–C bonds, which are essential in pharmaceuticals, agrochemicals, ligands for catalysis, and advanced functional materials. The first catalytic hydrophosphination (HP) was reported in 1990 with a platinum-based system[1] and since then the field has been largely driven by transition-metal complexes. However, recent advances have underscored the promise of main-group catalysts—especially crown ether–stabilized alkali metal phosphides—as more economical and environmentally sustainable alternatives. In this work, we employ density functional theory (DFT) to investigate the catalytic hydrophosphination of alkynes mediated by crown ether–stabilized alkali metal diphenylphosphides, AM(crown)PPh_2 (AM = Li, Na, K, Rb, Cs). The focus of our study is to unravel the mechanistic pathway involving nucleophilic attack of the phosphide anion on the alkyne followed by proton transfer, and to understand how the identity of the alkali metal cation influences reactivity and selectivity. In particular, we aim to rationalize the experimentally observed trend where heavier congeners such as Cs display higher reactivity compared to lighter metals like Li. Furthermore, our study will explore the influence of crown ether structure by comparing saturated versus unsaturated crown ethers in order to assess how ligand design modulates cation–anion interactions and transition-state stabilization. This work aims to reveal how alkali metal identity and crown ether design control catalytic efficiency, providing guidance for developing selective and sustainable main-group hydrophosphination catalysts.

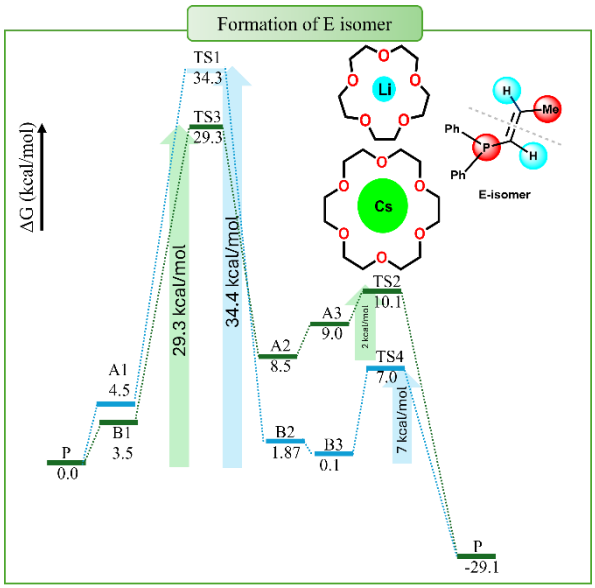


Figure 1 Energy profiles for alkyne hydrophosphination with crown ether–stabilized alkali metal phosphides. Cs exhibits the lowest barrier and highest reactivity compared to Li.

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Electronic Structure and Excited-State Properties of Covalently Bridged Diphenylhexatriene Dimers: Insights into Intramolecular Singlet Fission

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Singlet fission (SF) was first identified in anthracene crystals, where a high-energy singlet exciton (S_1) splits into two lower-energy triplet excitons (T_1).[1] This process has gained significant interest for organic solar cells and field-effect transistors. By generating two triplet excitons from a single absorbed photon, this process enhances light-harvesting efficiency and provides a route to surpass the Shockley–Queisser limit. In crystalline SF materials, crystal engineering plays a crucial role in intermolecular packing for loosely bound dimers, which is essential for efficient exciton splitting. However, in the case of covalently linked dimers, this reliance on crystal packing is eliminated. Intramolecular singlet fission (iSF) takes place when the singlet excited-state energy is at least twice that of the triplet state ($E(S_1) \geq 2E(T_1)$), and proceeds via a correlated ^{1}(TT) state to yield two triplet excitons. While the field of iSF has long been dominated by acenes, their relatively low triplet energies limit their integration with silicon-based solar technology. In 2023, Millington et al. investigated six isomeric diphenylhexatriene (DPH) dimers connected by a phenylene bridge and demonstrated efficient iSF with high triplet energies exceeding the silicon bandgap.[2] Two main mechanisms are proposed for iSF: a direct pathway and a charge-transfer (CT)-mediated pathway. In this work, we carried out a detailed excited-state analysis of DPH dimers using the Pariser–Parr–Pople (PPP) model within the Density Matrix Renormalization Group (DMRG) framework, DFT and TD-DFT.[3]

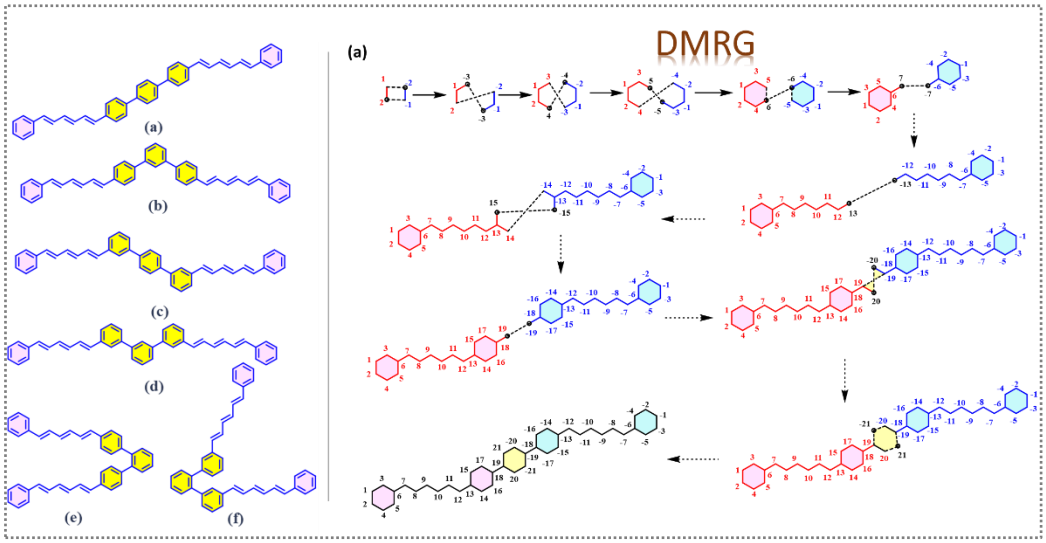


Figure 1 : Schematic representation of the molecules under study and the DMRG building scheme of molecule (a).

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Unraveling the Catalytic Activityof Mixed-Metal Conductive 2D MOFs for Water Splitting Reaction: A DFT Study

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Traditional catalysts used for the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in water splitting reaction have faced criticism due to their high cost and limited availability. To meet growing energy demands, it is essential to identify cost-effective and efficient alternatives[1]. Among various emerging materials, metal-organic framework (MOF)-based catalysts—particularly those free of precious metals—have gained significant attention. In particular, MOF composites featuring M–N–C or M–O–C (M = Fe, Co, Ni, etc.) active sites have shown promising catalytic properties for water splitting[2]. In this study, we employed periodic density functional theory (DFT)[3] studies to investigate the catalytic behavior of a conductive two-dimensional MOF system incorporating two single metal atoms centers as active sites. The studied systems comprises of two kinds of environment one is M-O-C site and the other is M-C site as shown in Figure 1(a) and different combinations of these two metal center are screened to identify the best one for OER/HER. Catalytic activity is analyzed based on the adsorption energetics of key reaction intermediates involved in the OER/HER reactions. Bader charge analysis is used to assess charge transfer characteristics and free energy changes of the elementary reactions are employed to construct free energy diagrams, from which the overpotentials associated with the OER/HER reactions are estimated. Among the systems studied, the Co–C site within the six-coordinate environment exhibited the highest catalytic activity, with a calculated overpotential of 0.39 V as shown in Figure 1(b).

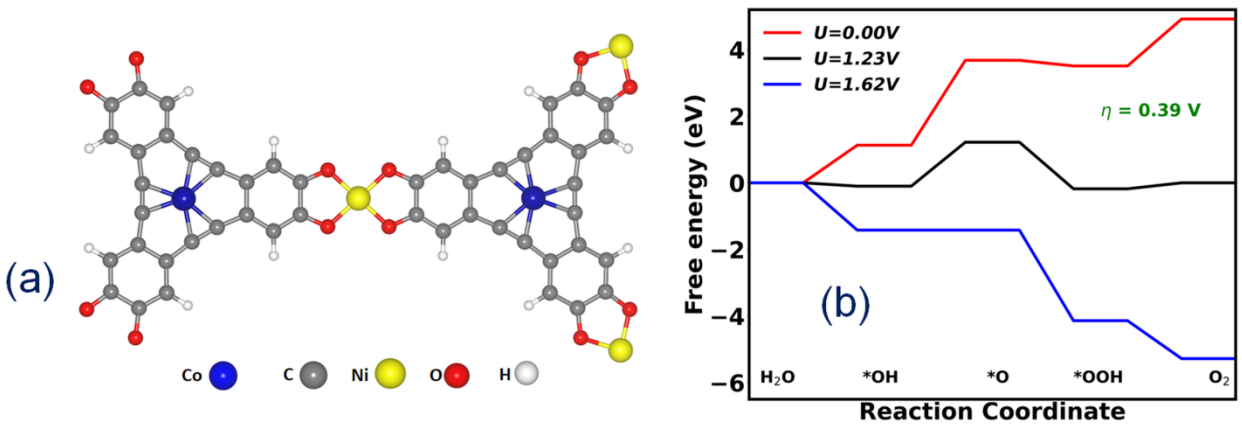


Figure 1 (a) Optimised structure of bare catalyst; (b) free energy profile for OER reaction.

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Trans-bent distortion of double bonds in heavier analogues of ethylene – Role of electron-sharing vs donor-acceptor bonds

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The reactivity of molecules is always related to their geometric structure. Therefore, reactivity can be fine-tuned by modifying the geometry either by intrinsic variations in the element or by using ligands with flexible electronic properties. The variation in structure and molecular properties of heavier main group compounds as compared to lighter analogues is example of the first category. The stabilization of low-valent main group compounds by electron donor ligands is a typical example of the second category. Such structural modifications often lead to unconventional bonding patterns. In this study, we examined how the structure and bonding pattern change when ethylene is replaced by its heavier analogues (E_2H_4, E = C – Pb). The ethylene is more stable in a planar geometry, whereas heavier analogues prefer trans-bent geometries. The detailed energy decomposition analysis, combined with natural orbital for chemical valence (using BP86/TZ2P level of theory in the ADF 2024.105 package), suggests that all planar structures favor electron-sharing E—E bonds, regardless of the group-14 element. Conversely, the trans-bent geometry of carbon (C) and silicon (Si) favors electron-sharing E-E bonding, while tin (Sn) and lead (Pb) analogues tend to favor donor-acceptor bonds. The Ge-Ge bond in the trans-bent geometry of Ge_2H_4 can be best represented by both electron-sharing and donor-acceptor interactions. The trans-bent geometries enable mixing of anti-bonding molecular orbitals formed by the interaction of sp hybrid orbitals with bonding molecular orbitals formed by the interaction p orbitals of main group elements. This four-orbital, two-electron interaction (see Figure 1) stabilizes as the main group element varies from carbon to lead, primarily due to increasing s orbital contribution in the sp hybrid orbital as the group progresses downward.

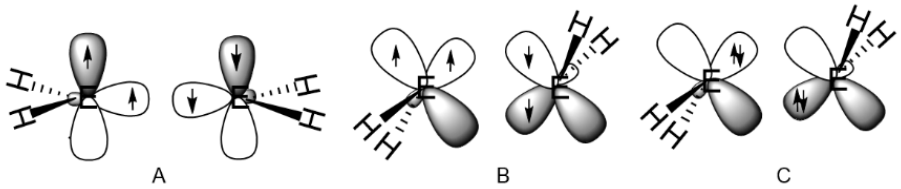


Figure 1 (A) Electron sharing bonding possibility in planar geometry (where E = C - Pb). (B) Electron sharing bonding possibility in trans-bent geometry (where E = C - Ge). (C) Donor-acceptor bonding possibility in trans-bent geometry (where E = Ge - Pb)

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Nitrogenase Inspired Nitrogen Reduction on Mo/Fe-Modified Subunene: A Computational Exploration of Bio-Mimetic 2D Catalysis

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Biomimetic catalyst design has attracted significant attention, particularly for ammonia synthesis, which remains challenging under ambient conditions. In this study, density functional theory (DFT) was employed to modify the subunene[1] framework into a single-atom catalyst (SAC) that emulates the Fe–Mo cofactor of nitrogenase. The tailored structure forms a cofactor-like environment through Fe–S and Mo–S coordination[3,4], enabling enhanced catalytic behavior. Fe- and Mo-doped subunene demonstrated remarkable stability, durability, and activity toward the nitrogen reduction reaction (NRR). The computational analysis revealed that the modified catalyst effectively inhibits the competing hydrogen evolution reaction while facilitating nitrogen adsorption. A detailed pathway investigation showed that nitrogen reduction proceeds efficiently across the sequential steps, with the Mo-doped system delivering outstanding catalytic performance and achieving an ultra-low overpotential of 0.04 V. These findings highlight the potential of subunene-based SACs as promising biomimetic catalysts for sustainable ammonia production, offering new insights into the rational design of efficient materials for NRR under mild conditions.

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Enhancing the power conversion efficiency of perovskite photovoltaics using a 3D/2D structure

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A combined material and device-related analysis is much needed to understand the working principle to explore the efficiency potential of triple cation-based Perovskite Solar Cells (PSCs). Therefore, here, density functional theory (DFT) and SCAPS-1D-based studies were reported to evaluate the photovoltaic (PV) performance PSCs. DFT is first applied to assess and extract structural and optoelectronic properties (band structure, density of states, Fermi surface, and absorption coefficient) of the considered absorber layer. Furthermore, to look for a suitable combination of the charge transport layer, a total of nine HTLs (Cu_2O, CuSCN, P3HT, PEDOT: PSS, Spiro-MeOTAD, CuI, V_2O_5, CBTS, and CFTS) and six ETLs (TiO_2, PCBM, ZnO, C_{60}, IGZO, and WS_2). Meanwhile, the crucial hurdle to commercialization is the 3D perovskite's instability. The development of bilayered (3D/2D) junction perovskites as light absorption materials has proven to be one of the most dependable approaches for stabilizing PSCs without compromising their power conversion efficiency (PCE) owing to the passivation capability of the massive organic cations. In this, the 3D/2D perovskites with optimized interfaces are developed by using a Ruddlesden–Popper (2D) phenylethylammonium lead iodide (PEA_2PbI_4) film on the top of a 3D triple-cation CsFAMAPbIBr perovskite and the device architecture is FTO/TiO_2/CsFAMAPbIBr/PEA_2PbI_4/Spiro-MeOTAD/Au. The effects of operating temperature, series and shunt resistances, Mott–Schottky, capacitance, generation and recombination rates, quantum efficiency, and current–voltage density were also examined by SCAPS-1D simulation[1]. The resulting PV properties were also compared with previously published data. Results reported in this study will pave the way for the development of high-efficiency solar cells in the future.

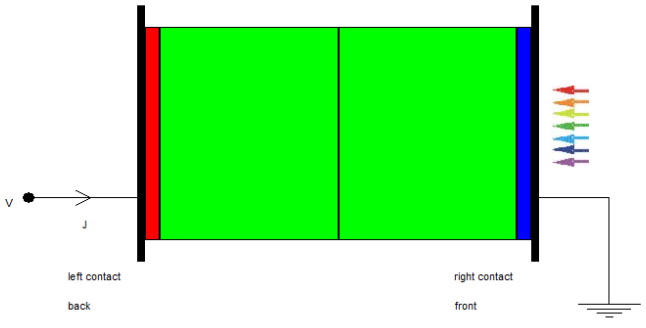


Fig. 1 Device Architecture(3D/2D)

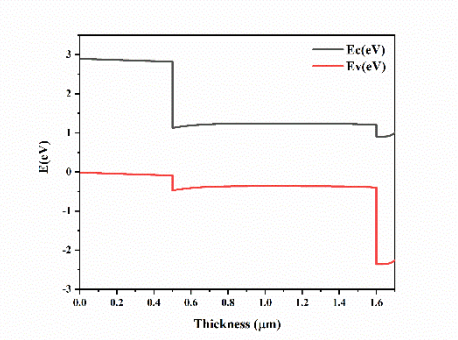


Fig. 2 Energy Band Diagram

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Structural and functional alteration of mutant DNA-binding domain of p53 protein in cancer

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Cancer is a genetic disease caused by a mutation in the genes associated with cell proliferation (proto-oncogenes) and apoptosis (tumor suppressor genes). p53 protein is a product of the tumor suppressor gene (TP53 gene). The p53 plays a key role in maintaining genome integrity. It detects DNA damage, and if the damage cannot be repaired, p53 activates the apoptosis (programmed cell death) pathway. To activate the pathway p53 protein's DNA-binding domain interacts with the DNA and activates transcription of genes responsible for apoptosis. Any mutation in the domain destroys its function and may lead to cancer. Here, we studied the M133T missense mutation using molecular dynamics simulations due to its pathogenic nature (CliniVar) and the amino acid change from a nonpolar to a polar residue (**Figure 1**). Our results suggest that during the simulation, protein surface area increases and interacts with the solvent with respect to the initial geometry, and specific fluctuations are observed in the loop region of the DNA-binding domain of p53 protein.

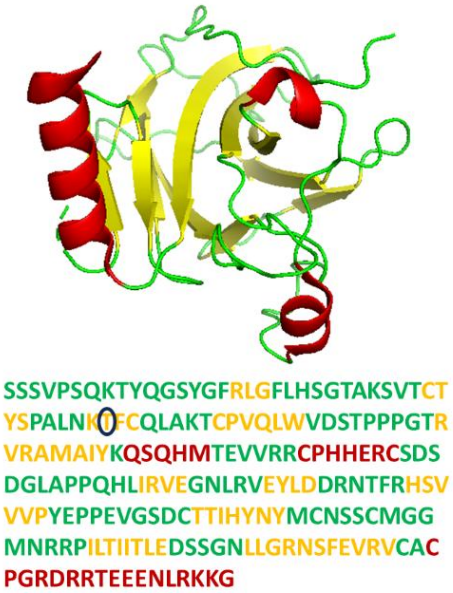


Figure 1 Structure of p53 protein

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Multi-Scale Modelling of Encapsulation Mechanism of Cyclam based Catalysts to Cucurbit-[8]-uril

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Cucurbiturils (CBs) are renowned supramolecular hosts with remarkable capacity for selective guest encapsulation in aqueous media, making them invaluable in host–guest chemistry. Cyclam, a macrocyclic tetraamine, displays broad utility in metal chelation, catalysis, and medicinal applications. Notably, its nickel complex (Ni-cyclam) is a benchmark electrocatalyst for carbon dioxide reduction. By forming host–guest complexes between CBs and cyclam (and its metal complexes), it is possible to harness and enhance their individual properties toward new advanced functions. In this study, the encapsulation energetics and complexation mechanism of cyclam and its metal derivatives with cucurbiturils were investigated using a synergy of computational approaches: molecular docking, molecular dynamics simulations, and well-tempered metadynamics. Structural and energetic analyses reveal that guest binding requires prior expulsion of cavity-bound water molecules, resulting in significant energetic barriers to encapsulation. Despite this, the hydrophobic character of cyclam derivatives substantially stabilizes the encapsulated complexes, favoring binding within the host cavity. The computed free energy landscapes present a comparative view of the complexation profiles for all guests examined, highlighting key insights into the balance of desolvation and hydrophobic stabilization governing supramolecular binding. This study lays the foundation for understanding and optimizing CB-based host-guest complexes for application in catalysis.

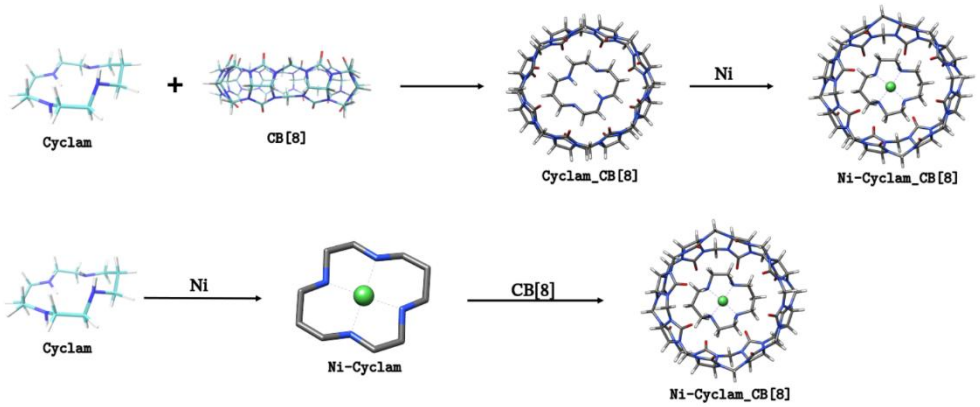


Figure 1 Possible pathways for the host-guest complexation

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Eumalanin Inspired 2D-Covalent Organic framework with a Porphyrin Core

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Eumelanin is a group of photoactive biopolymers that lack periodicity primarily due to the presence of multiple polymerization sites of the indole core[1]. One of the possible structural motifs believed to be present is the tetramer of indole framework arranged to form a porphyrin-like inner cavity [2]. To reduce the disorder in the polymeriztion pathways, we modelled the tetramer with the isostructural benzimidazole building block whose tetramer allows periodic extension to a rigid 2D material that can be rationally synthesized. DFT calculations on the tetramer shows a resilient framework capable of multielectron redox process. The extended 2D network formed from the tetramer shows (CGA/PBE at @440eV plane wave cutoff) a semiconducting indirect gap for the indole electron count, but a zero-band gap semiconductor with a Dirac cone[3] at Gamma when oxidized by two electrons. The presence of a porphyrin core in this framework allows facile metallation, allowing heavier metals to be employed to increase the spin orbit coupling assisted band-gap opening. In addition to the interesting photophysics generated by this bioinspired framework, the emergence of Dirac cone like features in the electronic band structure of benzimidazolecore could pave the way for applications in high-mobility charge transport, spintronics, and next-generation quantum devices. The frontier bands are dominated by aromatic sp^2 carbons, while the nitrogen lone-pairs lying low, resembling porphyrin. With the two carbon atoms originally holding a redox-active ortho-hydroxy/quinone couple available for substitution, this network provides substantial flexibility to tune its behavior by functionalization.

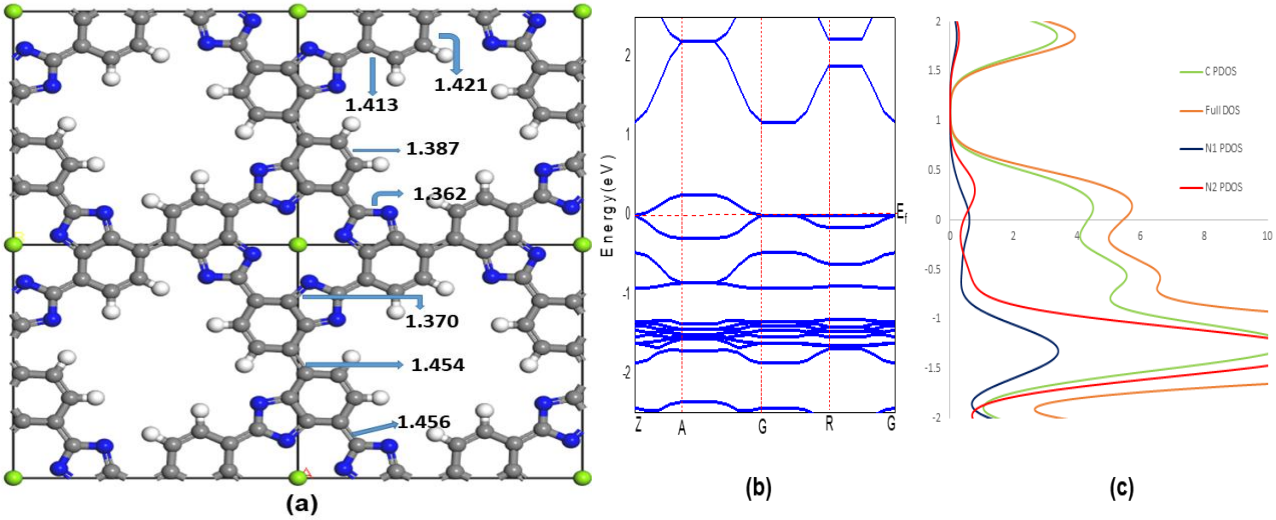


Figure 1 (a)The square p4 unit cell with magnesium metal at the center of the porphyrin core. (b) Electronic Band structure and (c)The Atom projected DOS

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SESMR: Overcoming the present-day challenges with hybrid classical-quantum computing approach

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Sorption-Enhanced Steam Methane Reforming (SESMR) is a two-in-one process that involves methane reforming with in-situ CO_2 capture and efficient blue H_2 production with enhanced yield[1]. However, microscopic insights into active sites, sorbent–catalyst synergy, and CH_4 activation remain limited due to the high computational cost of accurately modelling transition metal systems. Conventional DFT screening of these systems further suffers from inadequate electron correlation treatment and poor accuracy for d- and f-block elements, particularly when mapping diverse sorbent–catalyst–support combinations. Recent advances in quantum computing, an emerging technology, offer a promising pathway to address these challenges[2]. This work aims to overcome these challenges by introducing a hybrid classical-quantum computing approach and building a scalable framework in the field of catalysis research. As a starting point we investigate the properties such as binding energies of a tetrahedral Ni_4 cluster interacting with a CH_4 molecule. Using open-source python libraries such as PySCF, Openfermion etc, we optimised Ni_4, CH_4, Ni_4-CH_4 systems and mapped their fermionic hamiltonians to qubits using Jordan-Wigner transformation, which can be used to extract their energies by using quantum algorithms like Variational Quantum Eigensolver (VQE), Quantum Phase Estimation (QPE) etc, in a Quantum Computer. By this study we aim to demonstrate the potential for higher accuracy, faster convergence when compared to conventional approaches. By strategically benchmarking the energetics of several catalyst systems like that of Ni_4 cluster and gaining insights from them, we can bridge atomic scale precision with process level optimisation. This study serves as a proof of concept demonstrating how hybrid computing can accelerate the shift from classical simulation to quantum-empowered discovery in computational chemistry. Quantum technologies offer transformative power but face hardware, scalability, and stability challenges. Integrating quantum computing with AI and ML presents new opportunities to advance materials design, catalysis, and energy transformation research[3].

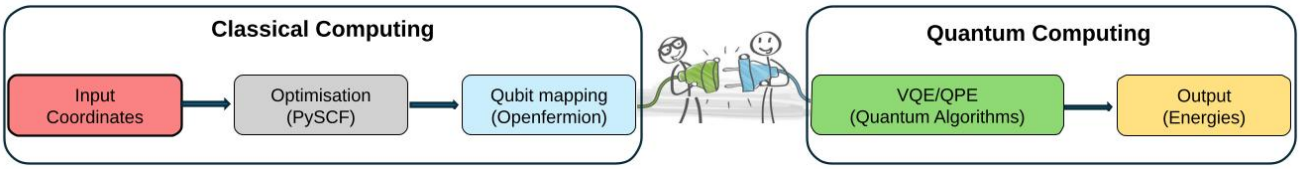


Figure 1: Hybrid Classical-Quantum Computing approach.

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Adsorption and Activation of CO_2 on Gold Grain Boundaries

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The electroreduction of CO_2 to CO, initially studied on the Au{111} planar surface, has been extended, in this project, to defect-rich surfaces to evaluate the role of grain boundaries (GBs) in catalytic activity. Experimental studies [1] indicate that GB terminations selectively enhance CO production while suppressing the competing hydrogen evolution reaction (HER), with activity scaling with GB density. To study what local atomic configuration drives such behavior, we systematically generated a library of 388 energy-minimized Au{111} grain boundary defect structures using coincident site lattice (CSL) methodology and energy relaxation in LAMMPS [2,3]. To capture topological diversity, we developed a novel screening framework, combining Gaussian isosurface representations with pairwise root-mean-square deviation (RMSD) comparisons, filtering redundant structures and identifying eight *distinct*, low-energy GB surfaces for detailed study. Ab initio calculations in CP2k were performed to optimize neutral-charge structures and determine favorable CO_2 adsorption sites and further validated by molecular dynamics simulations to account for thermally accessible configurations. CO_2 molecules were then adsorbed at high-occupancy, charge-rich sites across each GB. The activation criterion was defined as the surface charge density at which the chemisorbed CO_2 becomes energetically favored over the physisorbed state. Additional analyses were performed to characterize the local environment around each adsorption site and identify factors influencing the charge required to stabilize bent CO_2 on a given GB. This framework establishes a systematic link between GB topology and CO_2 stabilization and activation, enabling rational selection of defect-rich gold surfaces for CO_2 electroreduction catalysis.

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Effect of dispersion interactions on plasmon-induced hot carrier dynamics in metal NPs.

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Plasmonic nanoclusters (NCs), such as those of silver, have emerged as highly promising photocatalysts due to their ability to harvest light and generate excess energy (hot) carriers, which drive chemical reactions at the nanoscale. The energetic hot electrons and holes generated directly participate in photocatalytic reactions, enhancing activity and selectivity beyond what is possible with conventional metal catalysis. While there are a few works studying the effect of different exchange correlation functionals, to the best of our knowledge, there are no works studying the effect of long-range dispersion interactions on the plasmon-driven hot carrier generation. It is well-known that the inclusion of dispersion corrections brings changes to the structure and function of catalytic nanoclusters. Considering this aspect, in this work, we present a systematic study of how the dispersion correction affects both the structural and plasmonic properties of bare silver (Ag) NCs (Ag_{55}, Ag_{147}, and Ag_{309}), and on NCs interfaced with perfluorooctanoic acid (PFOA). Our results reveal that including dispersion corrections leads to changes in the absorption spectra and hot carrier generation profiles, both for bare and NC-PFOA systems.

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Fundamental Underpinnings of Ion-π Interactions: Essence and Nature

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Ion-π interactions, the noncovalent interactions between aromatic π-systems and charged species, have emerged as key contributors to a wide range of chemical and biological phenomena.[1,2] Both cation-π and anion-π interactions play critical roles in molecular recognition, catalysis, and structural stabilization.[1,2] Although these interactions are frequently rationalized in terms of the polarizability and quadrupole moment of the π-system, the (in)adequacy of such descriptors remains under active discussion.[3,4] The present study systematically examines the interactions of alkali metal cations (Li^+, Na^+, K^+) and halide anions (F^-, Cl^-, Br^-) with π-systems spanning both electron-rich (C_2H_4, C_4H_4, C_6H_6) and electron-deficient (C_2F_4, C_4F_4, C_6F_6) characters. High-level coupled-cluster calculations were employed to obtain accurate interaction energy profiles, which were subsequently decomposed into physically meaningful components, namely electrostatics, induction, and dispersion using symmetry-adapted perturbation theory.[5] We also evaluated the validity of widely used heuristic models, specifically the charge-quadrupole model for electrostatics, the charge-induced dipole model for induction, and the London equation for dispersion. The results indicate that, although the heuristic models remain valid in the long-range interaction regime, their validity diminishes as the ions approach equilibrium region or local minima. The study also reveals that, relying on the heuristic models to assess the energetics of ion-π interactions can lead to erroneous conclusions, as evidenced by the ability of some seemingly unfavourable interactions to produce metastable states and even bound states.[6,7] Overall, our study highlights the complexity of ion-π interactions and includes ongoing efforts to better understand these interactions at the fundamental level.

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Designing intramolecular singlet fission materials (iSF) with oligoacenes dimers: A correlated model Density Matrix Renormalization Group study

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Singlet fission (SF) is a promising method by which the Shockley-Queisser limit of solar cell efficiency can be superseded[1]. It has been long known that inter-molecular singlet fission (xSF) occurs in oligoacenes like tetracene and pentacene[1]. In xSF, one of the two adjacent molecules are photoexcited, and they interact with the a nearby molecule which is in the ground state to produce two low energy triplet excitons residing on the two adjacent molecules. Thus, improved inter-molecular coupling and packing arrangements are necessary to increase the SF efficiency which is not always possible[2]. Intra-molecular SF (iSF) is a process where the triplet excitons reside on the same molecule unlike the case of xSF where they reside on two neighboring molecules. Therefore, designing of iSF molecules can be a potential solution for increasing the efficiency of the solar cells[3]. In this respect, tetracene and pentacene dimers which are connected through phenylene spacer at ***para*** and ***meta*** positions and their electron donor substituted conformers (Figure 1) are crucial and calculations of the low-lying excited states are required to understand their photophysical properties. We employed Density Matrix Renormalization Group (DMRG) technique within the Pariser-Parr-Pople model Hamiltonian to study their low-lying excitations[4-5]. The DMRG calculations reveal that these oligoacene dimers satisfy the basic energetic conditions for SF i.e. [$E(S_1) \geq 2E(T_1)$] where $E(S_1)$ is the lowest dipole allowed singlet excited state of the dimer and $E(T_1)$ is the lowest triplet state of the monomer from which we can infer the possibility of iSF mechanism in them.

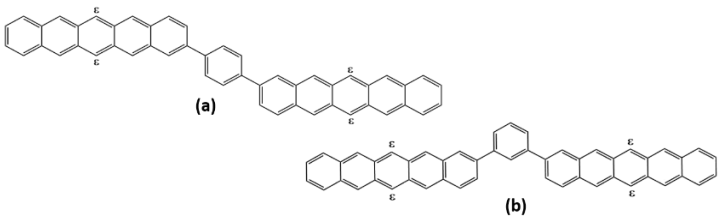


Figure 1 (a) *para*- (b) *meta*- substituted pentacene dimers.

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Theoretical Chemistry Symposium
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2D Si doped γ-Graphyne Monolayer as Potential Anode Material for Sodium-Ion Batteries

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In this study, we explored Si-doped γ-graphyne (SiG) system for applications in sodium-ion batteries (SIBs) using the density functional theory (DFT) modelling method [1,2]. AIMD simulations show that the system is thermodynamically stable at 400K. The system's dynamic stability is demonstrated via phonon calculations. Electronic property investigation reveals that the system is conducting and maintains its conducting behaviour after loading of Na-ion, as shown in Fig. 1(a). In the charge density difference study, it has been observed that Na-ion donates 0.88*e* of charge to the monolayer. During the adsorption of sodium-ion on various sites, it is seen that twelve-membered ring is the most stable site with an adsorption energy of -1.22 eV. Successive loading of Na-ion onto the monolayer indicates that 24 Na atoms could be stored over the 2 × 2 × 1 supercell of SiG monolayer as shown in Fig. 1(b), giving the formula unit as $Na_{24}C_{44}Si_4$. The system has the storage capacity of 1005.1 $mAhg^{-1}$. The convex hull is drawn using formation energies to get the stablest configurations. Moreover the voltage profile shows average working potential of 0.55V, which falls in safe range. These theoretical results confirm that the Si-doped γ-graphyne could function as a highly efficient anode material for SIBs.

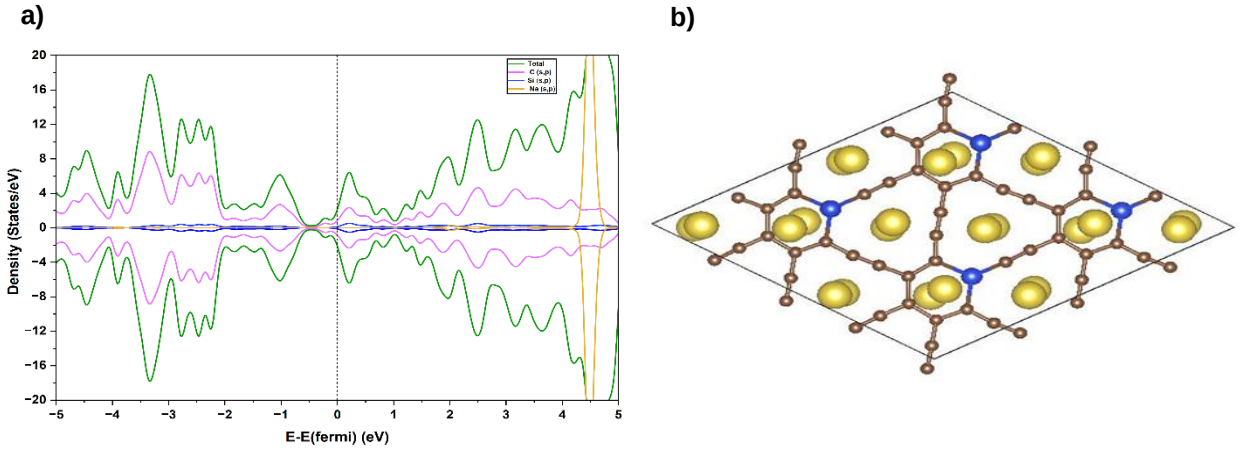


Fig.1 (a) Density of states plot for Na adsorbed SiG monolayer (b) Fully sodiated SiG monolayer. (Colour code: Carbon- Ochre, Silicon- Blue, Sodium- Yellow)

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Theoretical Chemistry Symposium
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Hydrophobic Collapse and Mechanical Forces in β-Hairpin Folding-Unfolding

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Proteins must fold into precise three-dimensional structures to function effectively. While much is known about the role of internal interactions during folding like hydrophobic collapse, the influence of very subtle forces[1] of the order of pico-newtons remains unexplored.

In this work, we employed molecular dynamics coupled with enhanced sampling to study the folding-unfolding of the TrpZip2 β-hairpin and the Small Protein under varying force conditions. Further we examined the effects of hydrophobic interactions, and external perturbations on the folding-unfolding pathway.

We converge to the conclusion that a force of ~5 pN along the backbone aids in stabilizing the native state, while deviation from this value destabilize the protein. The non-uniform forces from hydrophobic collapse, particularly of tryptophan residues, act as a natural directional pull guiding the backbone into its proper conformation[2]. Simulations with an external 5 pN force confirm that such a small pull is sufficient enough to bias the folding landscape toward the native state. We propose that tryptophan residues can exert an intrinsic force of this order on the peptide backbone. These insights suggest ways to design force-clamp experiments for stabilizing secondary structures.

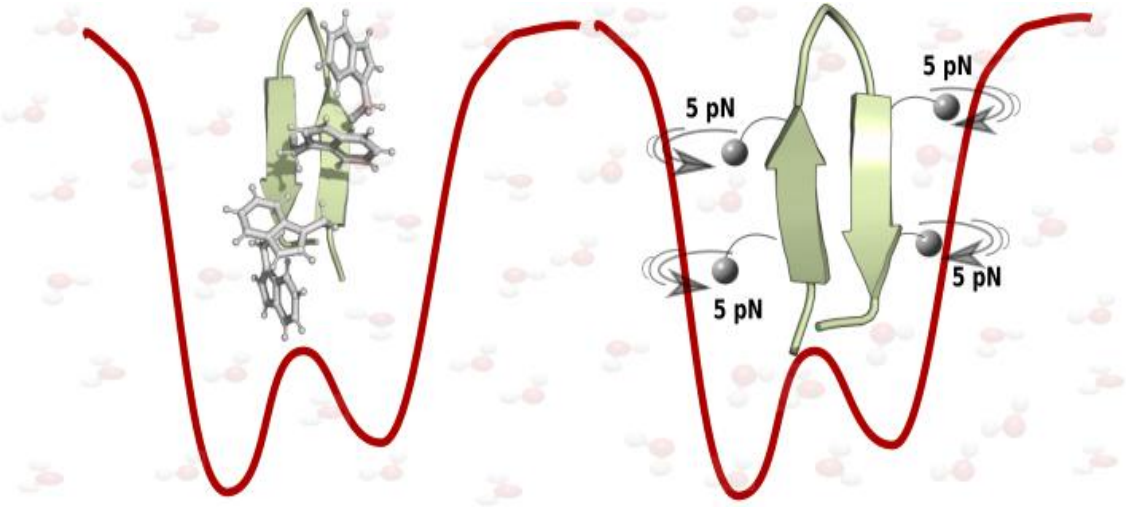


Figure 1 Free energy profile of a β-hairpin in the presence of tryptophan residues and under an applied 5 pN force.

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Theoretical Chemistry Symposium
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Finding the optimal position of substitution in Boranil-core for an efficient two-photon active photosensitizer – A case study

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Borate complexes that utilize an aniline-imine or salicylaldimine ligand, known as Boranil, exhibit several attractive properties, including excellent optical features, dual-state emission, a higher absorption coefficient, and a simpler synthesis pathway. Based on our literature review, we found no studies in which Boranil is used as two-photon (TP) active photosensitizer (PS) for two-photon photodynamic therapy (TP-PDT). Moreover, we identified a lack of systematic research regarding how substitution position affects the TP activity of Boranil. To address these gaps, we introduced iodine, dimethylamine, and six different polar groups at ten distinct positions on the Boranil core (shown in Fig. 1). As a result we designed total 48 systems for this work. In this study, we examined all mechanisms related to TP-PDT, including TP absorption (TPA), the rate of intersystem crossing, and the capability for singlet oxygen generation, using state-of-the-art RI-CC2 and DFT computational methods. Additionally, we investigated how our designed systems interact with human serum albumin (HSA) through molecular docking and molecular dynamics (MD) simulations. Our current work suggests that the substitution of iodine, dimethylamine, and the six different polar groups enhances the TPA strength of Boranil as well as our considered systems interact with the HSA carrier protein with favorable binding free energy.

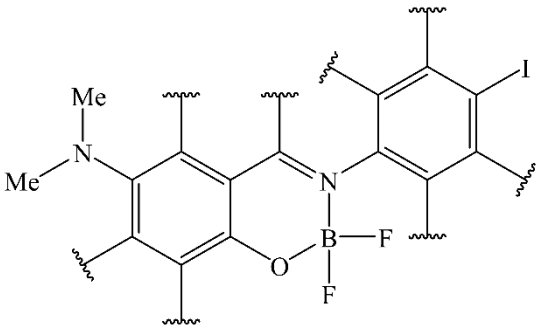


Fig. 1. Structure of Boranil core

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Selectivity and Switchability of Hot Spot Activation in Nanolens-like Nanosphere Heterotrimers

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Near-field coupling between metal nanoparticles creates regions of strongly confined electric fields at the junctions of the particles, known as hot spots[1]. Nanoparticle assemblies with multiple hot spots offer opportunities for optical control. Linear trimers of self-similar nanoparticles with a hierarchical arrangement of monomers in terms of particle size along the chain, often explored as nanolens configurations, focus electromagnetic energy in the vicinity of the smallest particle[2-5]. In contrast with the traditional nanolens configurations, the current study embarks on an exploration of the optical control of hot spots using nanolens-like trimers of nanospheres with compositional asymmetry and with a constant gap size using finite-difference time-domain simulations. We analyzed the optical control features of a plethora of dimeric and trimeric configurations by examining their electric field intensity distribution profiles at their extinction maxima. Of the six trimeric systems considered, two of them were found promising for achieving selective excitation of hot spots, while two others were found useful for accomplishing hot spot switching. For the systems demonstrating optical control features, a wavelength dependence study was conducted by exciting them at two commonly employed laser wavelengths, namely 457 nm and 633 nm. Our simulations[6] exemplify that a balanced choice of composition and size in the proposed nanolens-like configurations entails them with considerable optical control of hot spots, a prediction that is worth investigating in surface-enhanced spectroscopy experiments.

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Theoretical Chemistry Symposium
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Molecular Modeling of Amines and Amino Acid-based solvents for CO_2 capture : Predictive Parameters, Gaps and Challenges.

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The intensifying phenomenon of global warming has emerged as major environmental challenge. The mitigation of CO_2 emissions requires the development of efficient sorbents. Depending on the system, CO_2 capture involves either non-bonded interactions driving physisorption or bonded interactions controlling chemisorption. Identifying and quantifying the molecular parameters governing these mechanisms are essential to design efficient capture media which are often difficult to measure experimentally. Computational approaches, particularly systematically corrected-DFT (Density Functional Theory) protocols such as dispersion, solvation, thermal corrections etc., for accurate prediction of absorption energies, reaction enthalpies, activation barriers, charge distribution, and frontier orbital descriptors to assess thermodynamic and electronic characteristics of binding. These energetics will help to evaluate capture capacity, saturation loading and solvent regeneration, where excessively strong binding may hinder regeneration. While DFT-based thermodynamic cycles and solvation models often neglect explicit hydrogen-bonding effects, MD simulations address these limitations by providing insights into radial distribution functions (RDFs), hydrogen-bond dynamics, solvent accessible surface area (SASA), diffusion coefficients, free energy profiles, and structural stability. However, due to the reliance on fixed force fields limits the accurate description of polarization, charge transfer and chemical reactivity. Recent advances using ab-initio molecular dynamics (AIMD) and enhanced sampling overcome these limitations by computing interatomic forces directly from electronic structure and incorporate explicit solvation, enabling reliable predictions of bond formation, protonation equilibria and dominant species under realistic conditions.

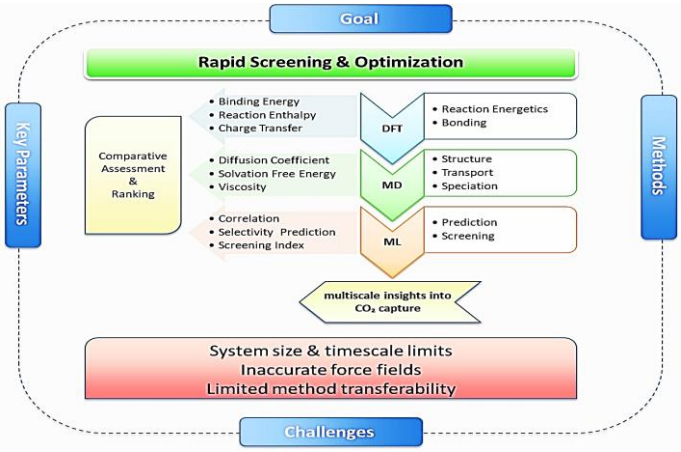


Figure 1. Multi-scale approaches for computational screening and optimisation of solvents.

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Beyond Aromaticity: What Really Controls NHSi and NHGe Reactivity with Diazoalkanes?

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Abstract: In this study, we present a comprehensive computational analysis of the reactivity of higher carbene analogues N-heterocyclic silylene (NHSi) and germylene (NHGe) with diazoalkanes, aiming to elucidate the mechanistic factors governing their divergent reaction pathways. Employing density functional theory (DFT) calculations in conjunction with the activation strain model (ASM) and energy decomposition analysis (EDA), we investigate two key reaction channels: C–H activation and N_2 extrusion. Our results demonstrate that aromatic stabilization significantly influences the overall reactivity trends; however, the pathway preference, particularly for the heavier analogues, is strongly affected by the deformation energy associated with the diazoalkane fragment. These findings highlight the interplay between aromaticity and structural strain in determining reaction outcomes.

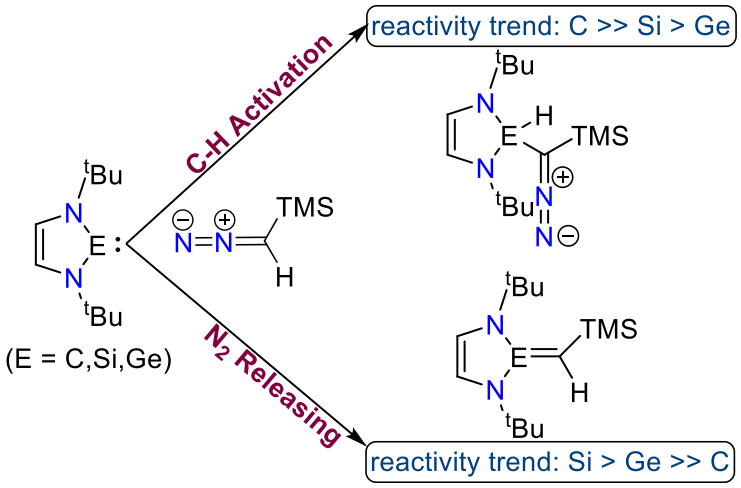


Figure 1. Replacing carbon with heavier elements (Si, Ge) in N-heterocyclic carbenes alters their reactivity with diazoalkanes, where a balance of aromaticity, strain, and fragment interactions controls the barrier heights.

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Theoretical Chemistry Symposium
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Development of in-silico models for phytochemicals present in ayurvedic formulation

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The study aims to develop in silico models for ayurvedic phytochemicals, mainly amalaki (*Phyllanthus emblica*), turmeric (*Curcuma longa*), and guduchi (*Tinospora cordifolia*), which can be used for computational drug design. These are the main components of Rasayanvati which is one of the ayurvedic formulations. The initial step is to parameterize the chemical system of ayurvedic phytochemicals in the CGenFF. Then, the developed parameters can be validated from the Cambridge Crystallographic Data Center (CCDC), where the developed parameters need to be tested for the reproduction of condensed phase properties. CCDC structures are generally the accurate representation of small crystal packing. The validation will also be done using molecular dynamics simulation. Once we get the validated parameters, we will extend our research to study their aggregation behavior and interaction with biological systems using molecular dynamics simulation. The proposed study offers practical solutions for treating some ailments for which ayurvedic remedies have shown promise but have not yet attained widespread commercial application.

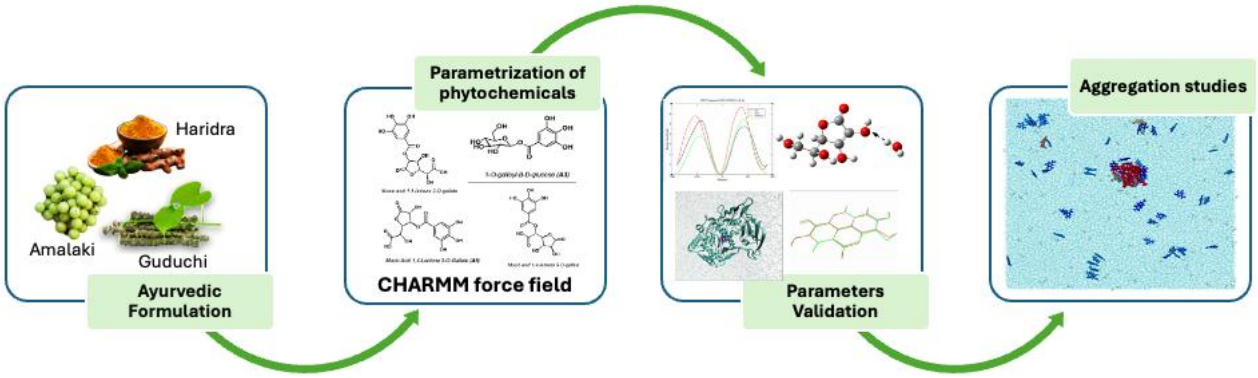


Figure 1 Parametrization of phytochemicals and their aggregation studies

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Theoretical Chemistry Symposium
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Theory for Inner Sphere Electron Transfer at Grain Boundary of Metal Electrode

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A semi-microscopic theory for anion bridge-assisted heterogeneous electron transfer, based[1] on the hypothesis that the transition state formed through the matching of the fluctuating quasi-Fermi level of metal with the fluctuating frontier molecular orbital of electroactive species, is developed. The extent of energy fluctuations required to form a desired quasi-Fermi state for ET over metal originates from solvent reorganization[2], anion adsorption, random nano-corrugated atomic steps[3] on single crystal hkl plane, grain and grain boundary density. Theory accounts for the effect of ion adsorption on the electrochemical work function, potential of zero charge, interfacial capacitance, electron affinity ratio, as well as on the standard rate constant for HET. The ion adsorption is governed by the partial coverage (θ_a) and the partial charge of adsorption (δ_a). δ_a is function of the electronegativity of ion, chemical hardness of ion and metal. θ_a is obtained from the Flory-Huggins adsorption isotherm[4] with microscopic modeling of the excess free energy of adsorption. Further, the free energy of activation ($\Delta G^{\neq}$) via bridging ligand complex for the ET kinetics is formulated as the product of the electron affinity ratio of electrode interface, and the energy gap between electrode and electroactive moderated through solvent reorganization. Theory accounts for the influence of ion adsorption, atomic steps, and grain boundary on ORR. Finally, theoretical predictions for the effect of anion adsorption on PZC and HET kinetics of complex ions, $[Cr(H_2O)_6]^{+2/+3}$, $[V(H_2O)_6]^{+2/+3}$ and $[Cd(H_2O)_6]^{0/+2}$ and also for the effect of grain boundary on work function and PZC show good agreement with the extensive experimental data for metal electrodes.

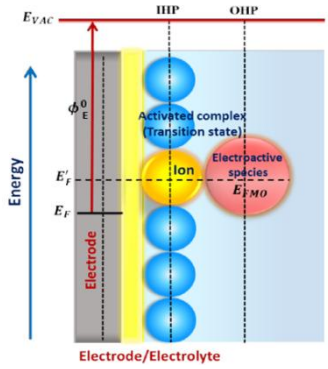


Figure 1 Schematic illustration of heterogeneous anion-bridge assisted ET occurring through the formation of quasi-Fermi state in metal jellium aligned with the fluctuating FMO of electroactive species.

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High-Throughput Discovery of Low-Valent and Linear Transition Metal CAAC Catalysts for Sustainable Nitrogen Fixation

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The exploration of small molecule activation using linear and low-valent transition metal CAAC complexes is an emerging area in catalytic science. Recent research[1] has demonstrated the promise of these complexes, such as the distinctive [(^{Et}CAAC)$_2$Fe] (CAAC=cyclic(alkyl)(amino)carbene) for effective nitrogen activation in homogeneous catalysis. Although various linear and low-valent transition metal CAAC complexes have been synthesized, their reactivity toward nitrogen activation remains largely unstudied due to the mechanistic details of nitrogen reduction reactions (NRR) facilitated by linear and low-valent transition metal CAAC complexes remain unknown and various factors like agostic interactions metal-ligand interaction affects the reactivity of these complexes. The complete mechanistic cycle exploration of N_2 activation (using static and dynamical caluations) by [(^{Et}CAAC)$_2$Fe] complex revealed that the most energetically demanding steps in the total catalytic cycle are the binding of dinitrogen to the catalyst and the reduction of the metal-dinitrogen complex.[2] Despite this uphill process, subsequent steps are also highly exergonic serving as the driving force for the overall conversion of N_2 into NH_3. Further, the comprehensive statistical analysis[3] of the parameters revealed the significant impact of metal-carbon bond distances and frontier orbital energies on catalytic performance. This study not only deepens understanding of NRR mechanisms but also informs the rational design of new catalysts, broadening the scope for their application in small molecule activation.

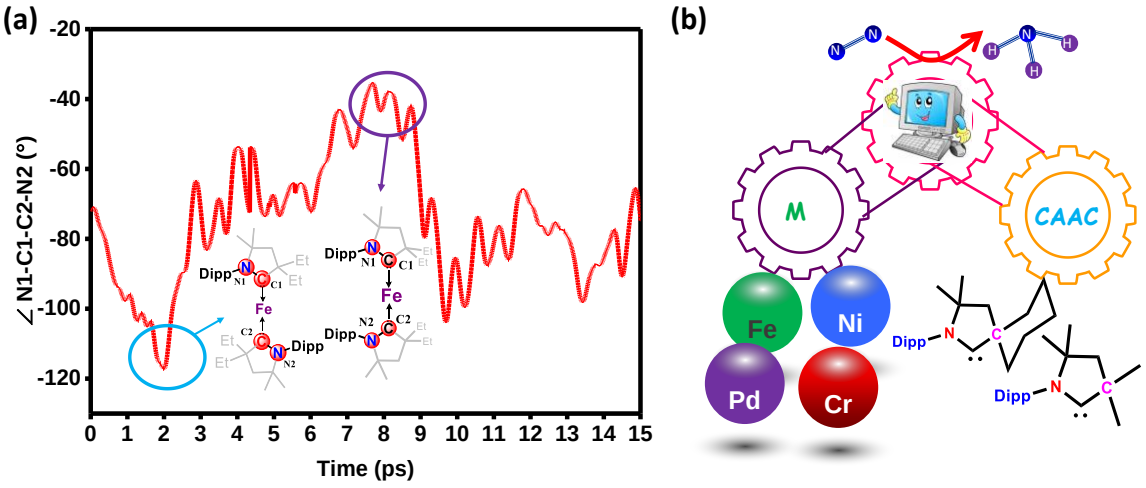


Figure 1: (a) ∠N1–C1–C2–N2 dihedral angle (in °) during simulation (b) High-Throughput Discovery of Low-Valent and Linear Transition Metal CAAC Catalysts for Sustainable Nitrogen Fixation

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From Genes to Membranes: Atomistic Simulations Reveal How GMGT Biosynthesis Shapes Archaeal Thermostability

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Abstract

The recent identification of archaeal enzymes catalyzing the biosynthesis and modification of glycerol monoalkyl glycerol tetraethers (GMGTs) has revealed previously unrecognized diversity in membrane lipid remodeling among extremophiles. While biochemical and genomic evidence implicates GMGT cross-linking and methylation in high-temperature adaptation, the molecular mechanisms by which these modifications modulate membrane properties remain unresolved. In this study, we propose to employ large-scale molecular dynamics simulations to systematically interrogate the structural and thermodynamic consequences of GMGT incorporation in archaeal membranes. By constructing atomistic membrane models of GDGTs and GMGTs with varying degrees of methylation and cyclopentane ring insertions, this study aims to quantify how these structural variants influence bilayer organization, fluidity, permeability, and mechanical resilience under extreme thermal and chemical conditions. Comparative simulations across lipidomes derived from Archaeoglobus fulgidus, A. profundus, and Vulcanisaeta distributa will establish links between genomic signatures of gms/gmm enzymes and emergent membrane behavior. This integrative framework will provide the first atomistic insight into GMGT-mediated homeoviscous adaptation, offering a molecular rationale for their evolutionary selection in hyperthermophilic archaea and informing the design of thermostable synthetic membranes.

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C−H Activation Initiated Skeletal Recasting of Cyclopropane Carboxylic Acid

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The selective activation of inert bonds remains a central challenge in organometallic catalysis. Here, we present a comprehensive mechanistic investigation of Pd(II)-catalyzed skeletal recasting of cyclopropane carboxylic acids, integrating C–H activation with strain-driven C–C bond cleavage. Using DFT at the SMD(HFIP)-MN15/def2-TZVP level, we explored multiple plausible pathways and identified the most energetically favorable route. The MPAA ligand plays a pivotal role in lowering the C(sp^3)–H activation barrier through a concerted metalation-deprotonation (CMD) pathway, while acetate-mediated CMD proved significantly less favorable. Oxidative addition of aryl iodide was revealed as the turnover-determining step ($\Delta G^{\ddagger}$ = 30.8 kcal mol^{-1} relative to I_2), consistent with experimental kinetics. Subsequent cyclopropane C–C bond activation and lactonization proceed via Pd(IV)/Pd(II) redox cycling, ultimately affording bicyclic lactone scaffolds. This study elucidates the cooperative roles of MPAA coordination, silver-mediated halide abstraction, and strain-release in enabling an energetically accessible catalytic cycle, offering insights into rational design of dual-activation strategies.

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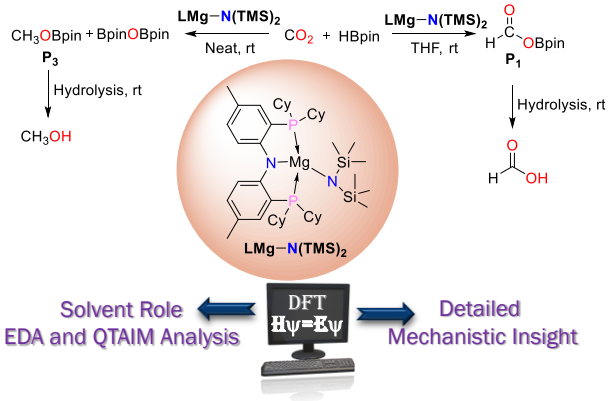
Solvent Controlled Pathways in Magnesium Catalyzed CO_2 Reduction to Formic Acid or Methanol: Insight from DFT Analysis

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The reduction of CO_2 into value-added chemicals remains a fundamental challenge in catalysis. This approach holds immense potential for creating cutting-edge methodology to utilize non-fossil-based materials. Recent studies by Rueping[1], Koley & Inoue[2], Okuda[3], and Westerhausen & Bontemps[4] have established that main group elements efficiently activate and reduce CO_2 and provide sustainable and cost-effective alternatives to transition-metal-based catalysis.

Experimental results reveal the striking solvent effect in Mg–PNP ligand catalysis(Scheme 1): in neat HBpin, CO_2 is fully reduced to methoxy borane (CH_3OBpin), whereas in THF solution, the reaction halts at boryl formate (HCOOBpin). Here, we present DFT-guided mechanistic details where solvent coordination plays the role of a “molecular switch.” In THF, Mg–solvent binding stabilizes a crucial intermediate and increases the barrier for subsequent reduction steps, redirecting the reaction to the formate product. Energy decomposition analysis demonstrates that energy barriers correlate with fragment distortion energies, revealing how solvent–catalyst interactions control CO_2 reduction selectivity and offering strategies for solvent-tunable catalysis design.

Scheme 1: Detailed work



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Efficient Machine Learning for Yield Prediction in a Transition Metal Catalyzed meta-C(sp2)–H Bond Activation Reaction

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The advances in catalytic C–H bond activation reactions, as well as that in the domain of machine learning (ML) has been unprecedented. In due cognizance of the potential of such technologies, we examine the utility of modern ML to predict the %yield of the transition metal-catalyzed meta-C(sp^2)–H bond activation reaction (m-CHA). The m-CHA dataset, comprising 866 reactions, curated manually from literature, highlights key characteristics of published reaction data, such as sparsity, structural diversity in substrates, reaction conditions, and imbalanced yield distribution. The Natural Language Processing (NLP) based transfer learning model (ULMFiT) , employing SMILES representation of molecules, is utilized for the yield prediction task. A novel pre-training dataset, denoted as SSP1, generated through a substructure-based sampling on the PubChem database, is introduced. The chemical language model (CLM) is found to extract equivalent chemical knowledge from SSP1 and ChEMBL datasets, despite SSP1 being only 8.5% the size of ChEMBL, providing a more time- and resource-efficient alternative. Further, we propose a new classification followed by regression (CFR) model for the prediction task to effectively mitigate the class imbalance inherent in the m-CHA dataset. The CFR model achieved a high accuracy of 90.25% using the DNN classifier and showed test RMSE values of 8.40±0.12 for the CFR-major class and 6.48±0.19 for the CFR-minor class with the ULMFiT-SSP1 regressor. Our CFR significantly outperforms direct regression (DR), in both m-CHA dataset and the commonly used HTE datasets. This work establishes CFR as a state-of-the-art method for yield prediction in sparse and imbalanced reaction datasets, offering a scalable and accurate approach to advancing reaction development and catalysis research.

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Uncovering the Unique Demeanour of Superatom Molecular Orbitals in C_{84} Derivatives

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Superatom Molecular Orbitals[1] (SAMOs) are atom-like orbitals that form diffuse hydrogenic excited electronic states of fullerenes, where the electron density is observed at the centre of the hollow cage. Discovering lower energy SAMOs gives a vital path to many electronic applications. This work through DFT reveals the SAMO states of C_{84} and endohedrally doped C_{84} derivatives with Sc, Ti, V, Cr, Mn, Fe, and Co atoms in molecular and periodic structures. A previous study with C_{80} revealed that the choice and position of metal atoms in the derivatives largely affect the orientation of SAMO energies and wavefunction distributions[2], which could also be observed with C_{84}. Opting for a higher fullerene derivative from C_{80} to C_{84} further reduced the SAMO energy, nearing the Fermi level. Among the different derivatives, Mn-substituted C_{84} comprises the lowest SAMO energy. The charge transfer also infers the influence of metal atoms in the cage on SAMO distributions. The overlapping of SAMO bands with higher dispersion bands among the higher energy values showcases the increased intermolecular interactions in the delocalized bands. Therefore, a higher fullerene derivative with lower SAMO energy opens up a new insight toward many charge transfer applications.

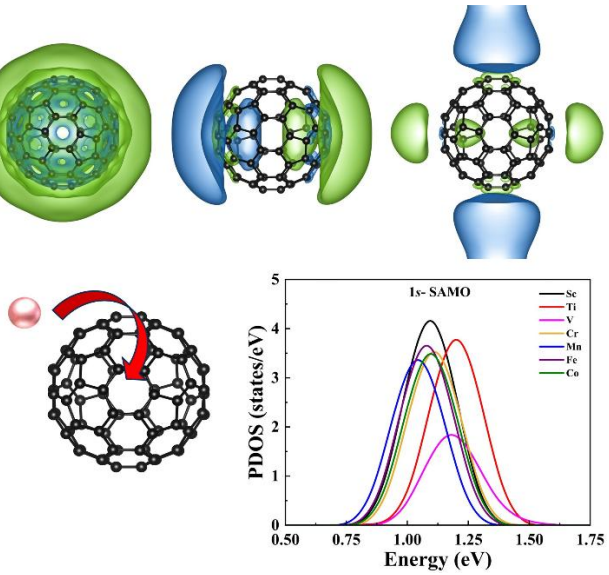


Figure 1 Representation of SAMO states of C_{84} and corresponding derivatives with their *s*- SAMO energies

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Quantifying the role of N-position in Imine based Covalent Organic Frameworks for Photocatalytic Water Splitting

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Photocatalytic water splitting offers a clean and sustainable pathway for hydrogen production. However, achieving overall water splitting remains a significant challenge due to the sluggish kinetics of the oxygen evolution reaction (OER), which requires a high overpotential. Recently, metal-free covalent organic frameworks (COFs) have emerged as a new frontier for photocatalysis, offering exceptional structural tunability for molecular-level active site engineering, broad visible-light absorption, and high surface areas that enable abundant adsorption sites. In this study, we propose a distinct OER mechanism wherein the process is initiated by thermochemical water dissociation, followed by electrochemical oxidation steps, offering a new perspective on overcoming OER limitation. Using first principle calculations, we have systematically designed and investigated fourteen distinct metal-free 2D COFs by tuning linker lengths and strategically incorporating nitrogen atoms at various positions within the linkers. Our results demonstrate that the thermochemical activation of water molecules at the nitrogen sites leads to protonation of the pyridine nitrogen atom, which in turn induces a push-pull electronic interaction with neighbouring carbon atoms. This interaction effectively lowers the energy barrier of the rate-determining step for both OER and HER, thereby enabling overall water splitting without the need for external bias. Furthermore, such protonation enhances charge transfer and π-delocalization across the framework, improving the photocatalytic efficiency. Importantly, our study highlights that the steric positioning and electronic configuration of N-atoms exerts a substantial influence on the electron density surrounding the catalytic centre. This effect, which has been rarely explored in a systematic manner, plays a critical role in stabilising the reaction intermediate and reducing the energy barrier of the rate-determining step. Our study provides key insight into how the steric location of the N-atom modulates the local electronic environment and catalytic activity of COFs, opening a new pathway to the rational design of high-performance metal-free photocatalysts for sustainable overall water splitting.

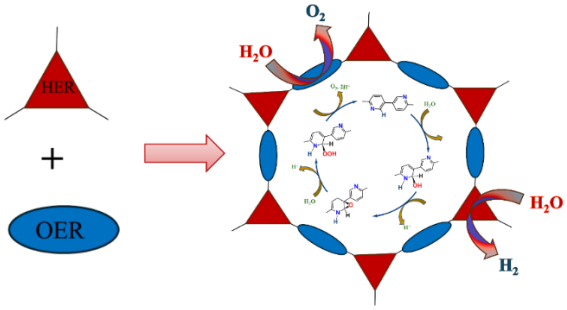


Figure 1. Schematic illustration of the studied Imine-based COF structures and their design principles**.**

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Computational Modelling of Single-Ion Magnet (SIM) on 2D surfaces : Hexagonal Boron Nitride and Graphene monolayer Surfaces

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Lanthanide-based single-ion magnets have received a lot of attention due to their great potential for storing information at the molecular level[1,2,3]. Individual magnetic adatoms on surfaces may exhibit long-lived spin quantum states and function as single atom magnets with significant remanent magnetization and coercivity at high temperature[4,5,6]. Inspired by prior works, we use periodic Density Functional Theory (pDFT) and multireference techniques to theoretically study the electronic structure and magnetization blocking of lanthanide atom/ion Dy, Dy(II), and Dy(III) adsorbed on a hexagonal boron nitride sheet (BNS) at four different sites and a graphene sheet at three sites. EDA and pDOS plots revealed significant interactions between adsorbed atom/ions and surfaces. CASSCF calculations including d- and p-shell electrons confirmed the presence of uniaxial magnetic anisotropy and effective anisotropy barrier suggesting the SMM behavior and enabling their application in advanced technologies.

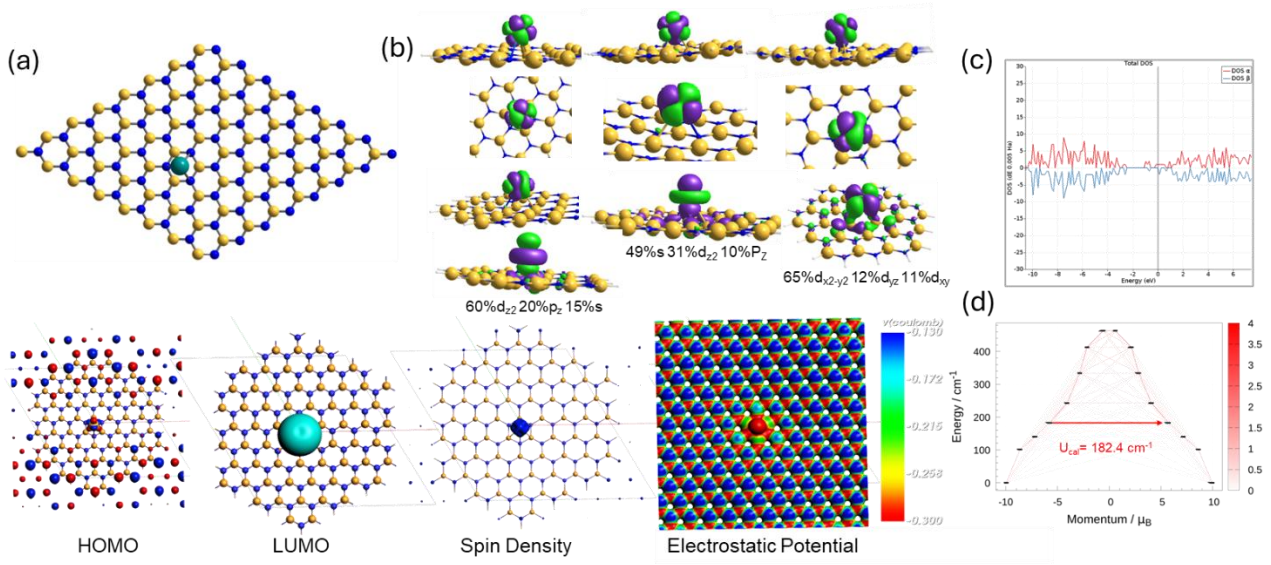


Figure: Adsorption of Dy(II) on (a) Boron Nitride sheet, (b) active space orbital of Dy(II) on BNS [CAS(10,10)], (c) pDOS of Dy(III) on BNS and (d) ab initio blockade barrier of Dy(III) on Graphene sheet.

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Computational Studies of Electrochemical Water Oxidation Reaction of Single-Atom Iron Catalysts

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Due to growing demand for energy and global environmental crises, there is an urgent need to develop green and sustainable solutions to produce clean fuel and chemicals, which replace fossil fuels and reduce carbon dioxide emissions. In this regard, electrochemical water oxidation reactions play a significant role in sustainable energy storage and production. Single-atom catalysts (SACs) in particular have great attraction, yet the influence of metal loading and coordination environment on their stability, reactivity, and tunability remains unclear. While much experimental research has been done for better electrocatalyst design for OER, a thorough understanding of the catalysts under explicit electrochemical conditions is missing. Keeping focused in this direction, we have studied the number of anchored iron atoms from single to multiple metal atoms over the graphene surfaces to evaluate the reaction free-energy profiles. It is found that the single-atom iron catalyst exhibits the lowest overpotential, which is consistent with d-band centre and DOS calculations. Grand-canonical-based quantum mechanical calculations are preferable to the computational hydrogen electrode method in evaluating the potential effect. A well-known Fe-NC material is a model system to build an electrochemical model for DFT calculations to understand the role of the electrochemical potential and electronic structures analysis.

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Molecular Modeling of Amines and Amino Acid-based solvents for CO_2 capture : Predictive Parameters, Gaps and Challenges.

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The intensifying phenomenon of global warming has emerged as major environmental challenge. The mitigation of CO_2 emissions requires the development of efficient sorbents. Depending on the system, CO_2 capture involves either non-bonded interactions driving physisorption or bonded interactions controlling chemisorption. Identifying and quantifying the molecular parameters governing these mechanisms are essential to design efficient capture media which are often difficult to measure experimentally. Computational approaches, particularly systematically corrected-DFT (Density Functional Theory) protocols such as dispersion, solvation, thermal corrections etc., for accurate prediction of absorption energies, reaction enthalpies, activation barriers, charge distribution, and frontier orbital descriptors to assess thermodynamic and electronic characteristics of binding. These energetics will help to evaluate capture capacity, saturation loading and solvent regeneration, where excessively strong binding may hinder regeneration. While DFT-based thermodynamic cycles and solvation models often neglect explicit hydrogen-bonding effects, MD simulations address these limitations by providing insights into radial distribution functions (RDFs), hydrogen-bond dynamics, solvent accessible surface area (SASA), diffusion coefficients, free energy profiles, and structural stability. However, due to the reliance on fixed force fields limits the accurate description of polarization, charge transfer and chemical reactivity. Recent advances using ab-initio molecular dynamics (AIMD) and enhanced sampling overcome these limitations by computing interatomic forces directly from electronic structure and incorporate explicit solvation, enabling reliable predictions of bond formation, protonation equilibria and dominant species under realistic conditions.

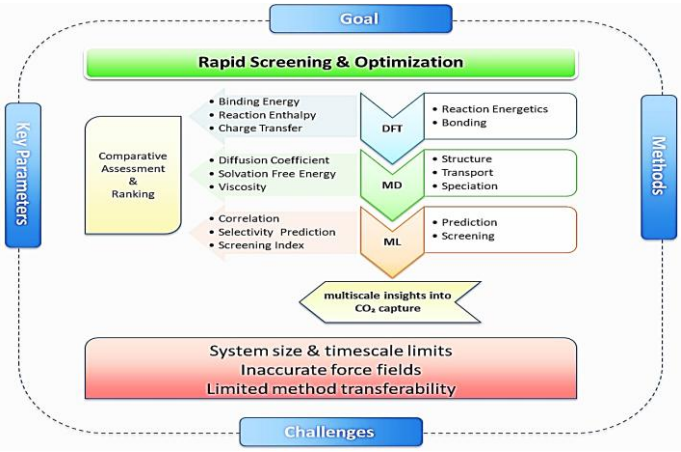


Figure 1. Multi-scale approaches for computational screening and optimisation of solvents.

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Target search dynamics of protein with varying flexibility and interactions of DNA backbone

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Target search processes are fundamental to several biophysical systems, enabling critical molecular events such as gene regulation, genome editing, and cellular signaling. Our research primarily concentrates on target search processes, especially the mechanistic aspects of the DNA-Protein target search problem. These processes often involve DNA-binding proteins locating specific target sites with remarkable speed and precision, despite the vast search space. The critical step for such events is thought to be a strategy called *facilitated diffusion*[1,2] which combines one-dimensional sliding along the DNA backbone with three-dimensional or bulk diffusion. The dynamics of the target search process is governed largely by the intricate interplay between protein–DNA interactions and the structural flexibility of the DNA backbone[3]. In our current work, we employ coarse-grained Molecular Dynamics (MD) simulations to investigate how variations in DNA backbone flexibility and non-specific interaction strength influence the target search dynamics of a diffusing protein. Using a Mean First Passage Time (MFPT)[4] approach, we aim to compute the timescales of 1D, and 3D motion executed by the diffusing protein and thereby the rate of the target search process.

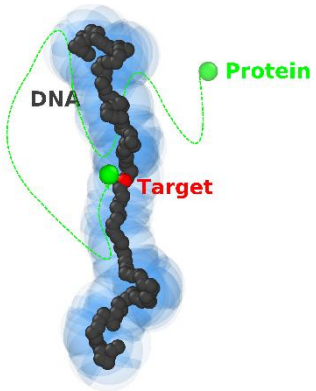


Figure 1 Schematic snapshot of a typical DNA protein target search process with protein as a spherical bead and DNA as a bead-spring polymer with the target at the centre and field of interaction (sky blue).

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Simulating Core-electron Spectroscopy of Liquid Water

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The core-electron binding energy (CEBE) provides information about local environment, which helps distinguish the hydrogen bonding network in ice clusters, surface water and bulk water. Experimental investigation of core-electron properties of liquid water from year 1986-2023, reports value in the range 1.3-2.8 eV, reflecting the challenges and discrepancies in experimental determination. This highlights the need for theoretical benchmark data on core electron spectra of liquid. However, due the need to describe many-body effects and associated high computational cost for describing the electronic structure for large number of solvent molecules, it becomes very challenging theoretically as well. We use static Coulomb-hole screened exchange (st-COHSEX), a post-KS method, for describing the many-body polarization effects in an efficient manner. To establish the accuracy of st-COHSEX method systematic study on basis sets and benchmarking against EOM-CC methods has been done. We discuss the role of density-driven errors on CEBE shifts and appropriate solutions to overcome the issues. Our study reveals for the first time that the bulk and surface water molecules have two distinct CEBE shift of O_{1s} compared to experimentally unresolved single peak. We also studied the structural differences of h-bonding networks in surface and bulk water that may attributes to different CEBE.

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Decoding Dynein's Mechanochemical Cycle Through Structure-Based Modeling And Atomistic Simulation

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Dynein is a molecular motor that converts chemical energy from ATP hydrolysis into mechanical motion. It consists of six AAA+ domains arranged in a ring, with the primary ATPase site (AAA1) located ~30 nm from the microtubule-binding domain (MTBD). The coordination between ATPase activity and microtubule (MT) binding is key to dynein's stepping mechanism, but the direction of this regulation remains unclear.

In this study, we used structure-based modelling[1] (SBM) to reconstruct the conformational transitions between pre- and post-powerstroke states. Additionally, we performed all-atom molecular dynamics (MD) simulations to explore MTBD behavior during stepping.

We observed a sequential transition in the AAA+ ring, where the domain rearrangement depends on the motor's powerstroke state. We also identified key intermediate states during the powerstroke cycle. Notably, AAA4 and AAA5 cooperate to produce stalk sliding, which regulates the MTBD's shift between strong- and weak-binding registries. This registry switch is facilitated by the presence of the microtubule. Without MT engagement or stalk motion, registry switching becomes energetically unfavorable[2].

Furthermore, we identified a conformational bottleneck when mutations render AAA3 or AAA4 inactive. These disruptions significantly impact the overall mechanochemical cycle, pointing to their potential role in regulating AAA1 activity.

Our findings offer a detailed view of how dynein integrates mechanical and chemical events and highlight key structural components responsible for efficient stepping.

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Mechanistic insights into the photoredox cyclopropanation of alkene with active methylene compounds

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Owing to the significant angle strain, rigid conformation and enhanced π-character of its bonding electrons, the cyclopropane ring stands as a prototypical strained system.[1] Their inherent ring strain makes them susceptible to ring-opening reactions, posing a significant synthetic challenge. The reaction scheme of photoredox catalysis in conjunction with active methylene compounds stands out as one of the most sustainable methods for constructing cyclopropane rings from alkenes (Figure 1).[2] With the aid of computational tools and techniques, we delineate the mechanistic landscape of the visible light induced, iodine and oxygen mediated cyclopropanation of olefins with esters, catalyzed by the organic photocatalyst 4CzIPN, under aerobic conditions.[3] Our findings highlight a cascade of single-electron transfer and radical coupling events accompanied by the cooperative effects of singlet and triplet molecular oxygen species. The intrinsic electronic and structural features of the C-C bond formation and selectivity determining transition states were analysed by employing spin density and natural bond orbital (NBO) analysis.

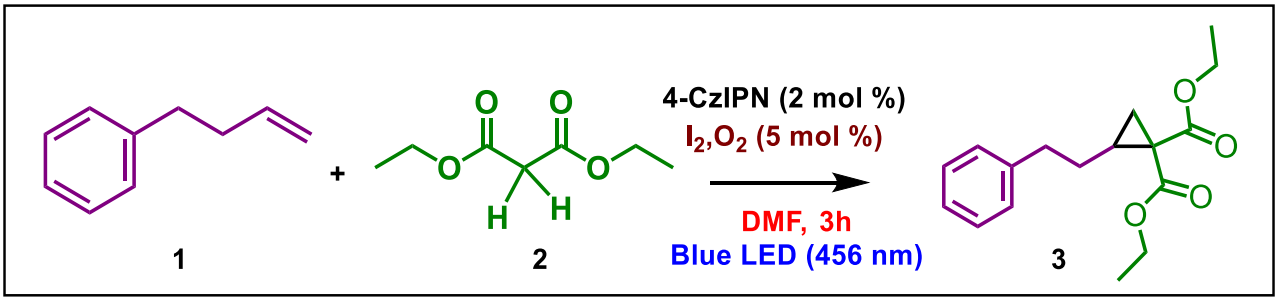


Figure 1 Photocatalytic cyclopropanation of olefins with active methylene compounds under blue-light irradiation.

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Unveiling the Mechanisms of Excited-State Formation in Radical-Based Organic Light-Emitting Diodes

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The emission in radical-based organic light-emitting diodes (OLEDs) originates from a spin doublet state rather than singlet or triplet excitons. In these OLEDs, the emission process is spin-allowed, circumventing the limitations imposed by triplet excitons.[1] However, some radicals typically exhibit low optical absorption and photoluminescence yields while others very emissive through the lowest first excited doublet state (D_1), making it crucial to understand the underlying mechanisms of how D_1 state is reached from the doublet ground-state (D_0) and establish design principles to enhance the absorption and luminescence yields of radical emitters.[2] Although previous studies have investigated certain processes contributing to D_1 formation[3], to the best of our knowledge, no simulations of the complete pathway from D_0 to D_1 have been conducted yet. In this study, we investigate three commonly used radical emitter molecules: TTM-1Cz, TTM-3NCz, and TTM-3PCz. These molecules share a common core structure of tris(2,4,6-trichlorophenyl) methyl (TTM) and contain varying carbazole (Cz) moieties. Using Marcus theory at the density functional level of theory (DFT), we compute the energy landscapes and barriers for multiple competitive pathways leading to D_1 formation. We also examine the validity of Marcus theory for such complex systems, particularly in regimes where quantum effects such as tunneling may become significant, especially in the inverted Marcus regime. The pathways analyzed include: i) D_1 formation via radical-anion intermediate, ii) D_1 formation via radical-cation intermediate, iii) D_1 formation via charge-charge annihilation, and iv) D_1 formation via higher-lying doublet or quartet states.[4] This in-depth DFT-based analysis of competitive pathways provides critical insights for designing next-generation radical emitters with improved efficiency and performance.

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Stochastic Logistic Growth Equation: Inhomogeneous Fluctuation-Induced Extinctions

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We study the stochastic logistic growth equation, which mathematically models the biological growth patterns of natural populations. While the general properties and stability analysis of the deterministic process have been well understood, less known are observables related to the stochastic level crossing, such as the first passage time and the escape probabilities through predefined targets. In this work, we thoroughly analysed the influence of fluctuations on the completion rates and associated probability factors. We observe that the growth rate fluctuations cause the independent population trajectories to approach the extinction limit beyond a certain threshold of the noise strength. We determine the conditions that predict a population's extinction or outbreak, as well as the related timescales. This stunning observation instils the further study that explores the possibility of any noise control mechanism (harvesting or resetting) that can delay or accelerate the extinction process.

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Computational Discovery of B–Al–Ga Nanoclusters for Oxygen Reduction Reaction Catalysis

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Abstract: The search for efficient catalysts is central to the progress of renewable energy technologies, particularly fuel cells. Platinum still sets the benchmark for the oxygen reduction reaction (ORR), yet its scarcity and cost remain serious drawbacks. In this work, we applied a computational strategy combining global structure searches with conceptual density functional theory (cDFT) descriptors to investigate boron–aluminium–gallium (B–Al–Ga) nanoalloys. From an extensive set of candidate clusters, a number were shortlisted and then examined in detail through adsorption energy calculations, solvation corrections, and ab initio molecular dynamics simulations. Among these, two clusters, B_4Al_2 and B_2Al, were identified as promising, showing moderate overpotentials and good stability even under solvated conditions. Examination of their electronic features reveals the composition–activity relationships, where boron facilitates stability and electron uptake, aluminium contributes to higher reactivity, while gallium fine-tunes electron donation. Taken together, these results suggest guiding principles for the design of platinum-free ORR catalysts and illustrate a general computational framework that can be applied to other catalytic systems in the search for sustainable materials.

Figure 1: Overpotential Values for Binary and Ternary Clusters

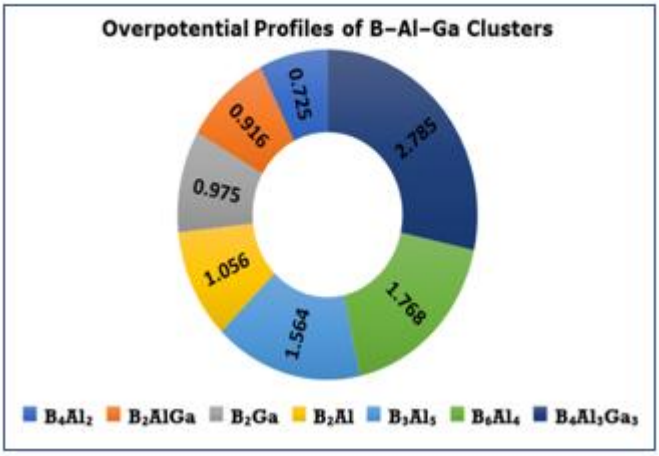
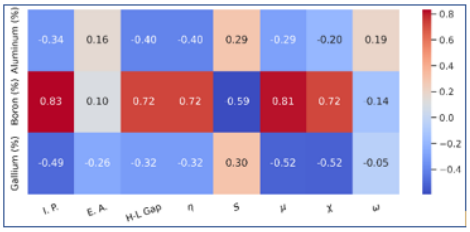


Figure 2: Correlation Matrix for Properties and Element Percentage



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Theoretical Chemistry Symposium
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Efficient Propagation Schemes for the Time-Dependent Schrödinger Equation in Strong Magnetic Fields: From Classical Integrators to Emerging Data-Driven Approaches

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The accurate and efficient solution of the time-dependent Schrödinger equation (TDSE) remains a central challenge in molecular quantum dynamics, particularly under **strong magnetic field conditions**, where non-perturbative interactions, Landau quantization, and anisotropic couplings introduce severe numerical instabilities. Traditional grid- and basis-based approaches require propagators that balance stability, accuracy, and computational efficiency across long time scales.

We compare the **performance and efficiency** of widely used propagation schemes[1] — **Split-Operator (SO), Chebyshev expansion, Crank–Nicholson** and **Modified Cayley** methods—against **short iterative Krylov subspace** approaches such as **Lanczos** and **Arnoldi propagators**, as well as **Magnus expansion** techniques and higher-order exponential integrators. Each method offers distinct advantages: Chebyshev and Krylov schemes excel in stability for large sparse Hamiltonians, Magnus and exponential integrators provide systematic control of time-ordering effects, while SO methods remain attractive for their simplicity in separable Hamiltonians. In strong magnetic fields, the vector potential couples momentum and position, breaking separability, increasing stiffness, and requiring adaptive or higher-order propagation schemes to prevent numerical diffusion and phase errors. Careful selection of the propagation method under such constrained environments is therefore crucial to ensure stability, accuracy, and computational efficiency.

Looking forward, data-driven approaches such as **Physics-Informed Neural Networks (PINNs)** [2], **Fourier Neural Operators (FNOs)** [3], and **Deep Operator Networks (DeepONets)** [4] offer promising future directions. By embedding the Schrödinger operator and magnetic field constraints directly into their frameworks, these methods provide mesh-free scalability and potential advantages in tackling high-dimensional Hilbert spaces and parameter sweep in problems.

his work therefore motivates a systematic roadmap: benchmarking classical propagators for strong-field molecular dynamics, identifying their breakdown regimes, and exploring how emerging machine-learning–based solvers might extend quantum simulations into challenging magnetic environments of astrochemical interest.

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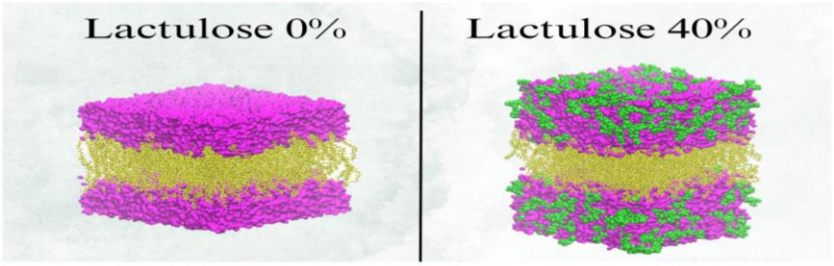
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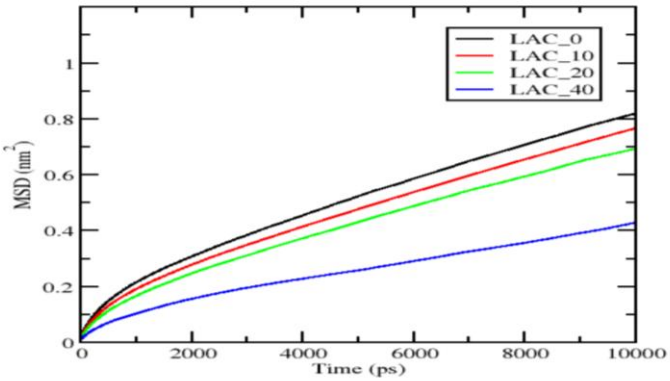
The Differential rigidity of lipid bilayers with varying lactulose concentrations reveled by All Atom Molecular Dynamics Simulations

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We used molecular dynamics simulations to investigate the concentration-dependent effects of lactulose on Dipalmitoylphosphatidylcholine (DPPC) bilayers. Systems with 0–40% lactulose revealed reduced area per lipid, increased interlamellar spacing, and denser bilayer packing. Density profiles showed lactulose associating with headgroups, reducing water penetration, while electrostatic analysis indicated enhanced bilayer barrier properties. Radial distribution functions confirmed strong phosphate-lactulose interactions at the expense of phosphate-water contacts. Lactulose increased acyl chain order, reduced lipid and water diffusion, and slowed collective headgroup and tail motions. Overall, lactulose stabilizes DPPC bilayers by strengthening headgroup interactions and restricting dynamics, offering molecular insight into carbohydrate-lipid interactions.





$$\langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_{i=1}^{N} \langle |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \rangle$$

References:
1. The Differential rigidity of lipid bilayers with varying lactulose concentrations reveled by All Atom Molecular Dynamics Simulations
P. P. Singh, C. Dey, S. Chakraborty* (Submitted)

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Molecular dynamics simulation of phase transition in lead-based perovskites

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Inorganic lead halide perovskites, $CsPbX_3$ (X = I, Br), have attracted significant interest in photovoltaic research due to their enhanced thermal stability compared to hybrid perovskites, primarily attributed to their fully ionic composition. The structural stability and phase transitions of these materials can be effectively investigated using classical molecular dynamics simulations; however, the accuracy of the results strongly relies on the force field parameters. In this study, we critically evaluate three previously reported force fields for the $CsPbI_3$ system and two force fields for the $CsPbBr_3$ system [1-3]. The performance of each force field is assessed based on its ability to reproduce bulk structural parameters, mechanical properties, and phase transitions. Our results highlight the importance of octahedral distortions, specifically the Pb-X-Pb bond angles, in governing phase transitions. Simulations show that force fields accurately capturing phase transitions display an increase in Pb-X-Pb bond angles with temperature, shifting the distribution towards higher values. In contrast, force fields failing to predict phase transitions exhibit the opposite trend. These findings suggest that phase transitions in $CsPbX_3$ are strongly dependent on the distortion of PbX_6 octahedra.

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In Silico Screening Reveals Natural Compounds from Ashwagandha, Haritaki, and Tilpushpi as Potential Inhibitors of Tumor-Promoting Ornithine Decarboxylase

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Ornithine decarboxylase (ODC) is a pyridoxal-5′-phosphate (PLP)-dependent enzyme that catalyzes the rate-limiting step in polyamine biosynthesis, a pathway strongly associated with cellular proliferation and tumorigenesis.[1] In this study, a curated library of 412 phytochemicals derived from 52 medicinal plants with known anticancer properties was screened in silico for drug-likeness, pharmacokinetic profiles, and binding affinity toward the ODC homodimer.[2] 130 compounds were subjected to molecular docking followed by ADMET filtering, which showed a total of 13 top compounds with high affinity. Furthermore, Molecular dynamics (MD) simulations over 100 ns confirmed stable binding for 9 top candidates, and MM-PBSA free energy calculations, along with per-residue decomposition analysis, highlighted 5 phytochemicals with superior binding profiles. Notably, Withanone, Withaferin A, and Withanolide D (Ashwagandha), Arjunic Acid (Haritaki), and Digitoxigenin (Tilpushpi) exhibited higher binding affinities than the known natural inhibitor Myricetin. These compounds engaged key residues within the ODC active site, potentially disrupting its catalytic function. Structural parameters such as RMSD, radius of gyration, and hydrogen bond persistence supported the dynamic stability of these ligand–protein complexes. Importantly, MD simulations revealed persistent water-mediated interactions in the active site, which may enhance binding affinity and contribute to inhibitory activity. These findings position selected phytochemicals as promising reversible ODC inhibitors and warrant further experimental validation in the future to explore their potential in anticancer therapy and in elucidating the mechanism of ODC inhibition.

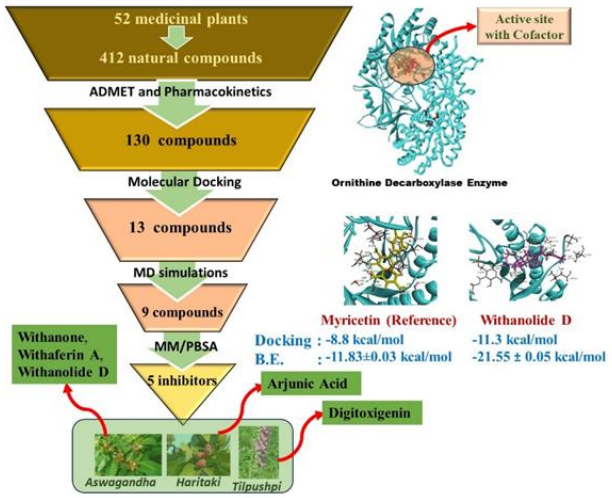


Figure 1: Screening methodology and identification of the natural compounds for ODC inhibition.

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Computational Insight Towards the Chemisorption of Toxic Carbonmonoxide by an Anti-aromatic COF

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Antiaromatic 4n π-electron systems have been looked up on lately with great importance owing to their high reactivity and low homo-lumo gap. They are predicted to have huge potential for energy storage materials and also being an organic compound adds to their value. But it has been a challenge to stably synthesize them. To this end, people have successfully synthesized and stabilized these compounds via annulation with aromatic (4n+2) π-groups. Also, covalently linking them and getting them to self assemble to form covalent organic frameworks (COF) has been yet another technique to stabilize these antiaromatic moities to form novel functional materials. Herein, with the help of the Molecular Dynamics (MD) simulations we assess the formation of the Dibenzopentalene (DBP) COF. Most importantly through our Density Functional Theory (DFT) calculations, we also introduce here for the first time the ability of these DBP COFs in effective chemisorption of the Carbon Monoxide (CO) and thus projecting a promising, novel material for the toxic CO capture.

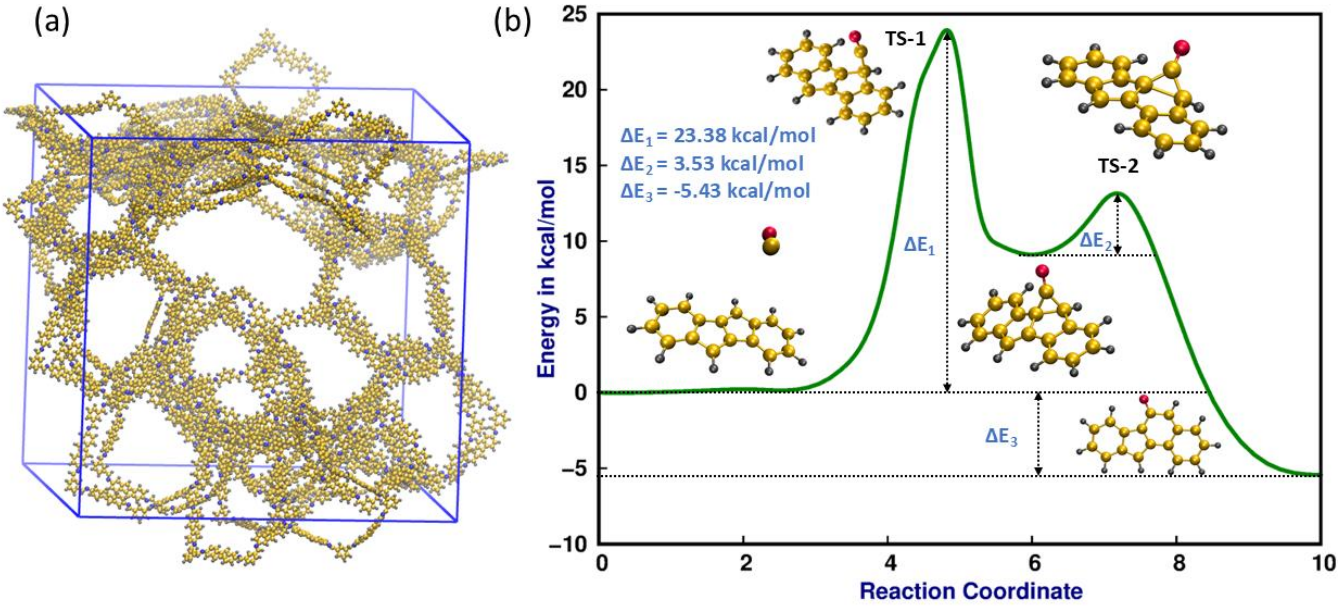


Figure 1: (a) Self-assembly of a macrocycle containing six anti-aromatic DBP units leading to the formation of a COF. (b) Affinity of the DBP moiety toward binding with toxic CO molecules.

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Computational Insights into the Operation of a Molecular Rotary Motor Driven by an Appel Reaction

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Kinetic asymmetry is a foundational principle for molecular machines, enabling the conversion of chemical energy into directed, unidirectional motion[1] by establishing differential activation barriers between forward and reverse reaction steps. This study provides computational insights into the operation of a recently reported phosphine oxide–phenol-based molecular rotary motor driven by an Appel reaction[2], a system that uses kinetic gating via a chiral alcohol to bias the reaction cycle. Using Density Functional Theory (DFT) at the ωB97X-D/6-31+g(d,p) level, we examined the complete 360º rotation mechanism, first analyzing the methyl-substituted analogue (**1c**) and then the actual motor (**1a**). The calculations confirmed that the chiral alcohol, (S)-1-phenylethan-1-ol, preferentially reacts with the atropisomer **3a** over **2a** by lowering the reaction barrier, which aligns with experimental results and introduces the necessary kinetic asymmetry to the cycle. Critically, the computational analysis reveals a significant difference in the atropisomer interconversion barrier (**2**⇌**3**) between the analogues. The hydrogen-substituted motor (**1a**) exhibits a substantially lower barrier (10.1 kcal/mol) compared to the methyl analogue (**1c**) (14.8 kcal/mol). This reduced steric hindrance in **1a** makes the **2a**⇌**3a** interconversion significantly more facile. Furthermore, the final rotational barrier (**1**⇌**4**) is drastically reduced from 41.0 kcal/mol in **1c** to 24.7 kcal/mol in **1a**. These findings demonstrate that the lack of the steric methyl group in the actual motor (**1a**) facilitates the key kinetic steps, thereby enhancing the overall efficiency and feasibility of the complete unidirectional rotary cycle. This computational work validates the kinetic gating mechanism and provides a detailed molecular-level understanding crucial for the future design and optimization of autonomously fueled molecular machines.

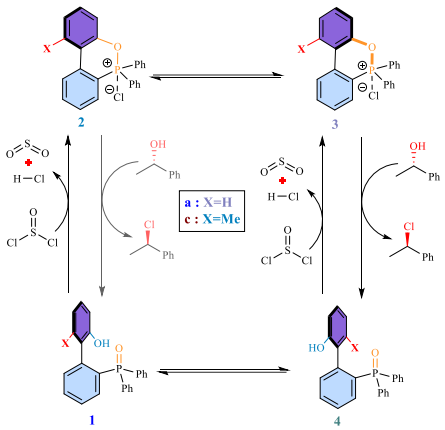


Figure 4 Chemical cycle of phosphine oxide–phenol- based molecular rotary motor.

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Role of Fluorination on the Excited State Dynamics of Methyl Salicylate: Insights from Surface Hopping Simulations

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Methyl salicylate (MS) is a well-studied molecule exhibiting excited state intramolecular proton transfer (ESIPT)[1,] and it is commonly used as a building block for photoprotective materials, such as UV filters and photostabilizers. To alter the properties, structural modification by substitutions, such as fluorination, offers a promising approach. Fluorination is widely employed to alter the excited state properties of conjugated aromatic systems as it affects the geometrical parameters and interatomic interactions[2.] In this work, we employed MP2, ADC(2), and CASSCF methods for structural evaluation, and trajectory-based surface hopping simulations at ADC(2) level for dynamics studies. We focused on the first two singlet states: the ground state (S_0) and the first singlet excited state (S_1). Our results show that fluorination induces non-planarity in certain isomers of MS in both the S_0 and S_1 states. In MS, PT is ultrafast, completing within 35 fs. Upon mono and tetra-fluorination(s), this time decreases to ~ 30 fs. Minimum energy conical intersection structures were explored, before and after PT. After 1.5 ps of dynamics simulations, we found that only ~ 10 percent of the S_1 populations decayed to the ground state, for both MS and mono-fluorinated MS. However, tetra-fluorination results in ~ 20 percent of population decay.

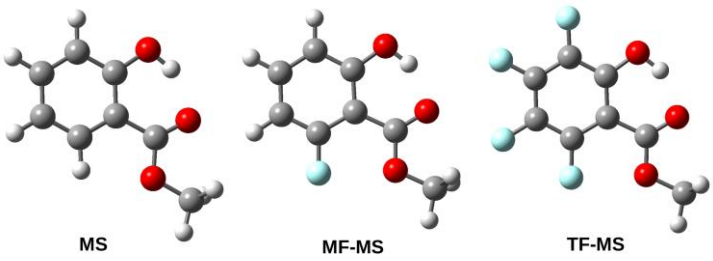


Figure 1: Optimized Structures of the Most Stable Conformers in MS, mono-fluorinated (MF-MS) and tetra-fluorinated (TF-MS) in S_0

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Cobalt Catalyzed Asymmetric Hydroacylation Reaction of 1,3-Dienes: Mechanism and Origin of Regio- and Enantioselectivities

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Abstract

Hydrofunctionalization of substituted diene yields a plethora of primary products, encompassing [1,2]/[2,1], [1,4]/[4,1], and [3,4]/[4,3]-adducts. Elucidation of mechanisms governing catalytic enantio- and regioselective transformation with substituted diene is often challenging. Herein, we provide mechanistic underpinnings derived through a comprehensive density functional theory (UB3LYP-D3) investigation, unraveling the origin of regio- and enantioselectivity in a Co-catalyzed asymmetric hydroacylation reaction involving 1,3-dienes and *iso*-propyl aldehyde.[1] The energetically preferred pathway proceeds through a) the generation of an active catalyst [(*S,S*)-Ph-BPE)Co^{I}]$^{+}$$BARF^{-}$ in singlet spin state, achieved via Zn reduction of precatalyst [(*S,S*)-Ph-BPE]$Co^{II}Br_2$ in the presence of NaBARF as an activator, b) an oxidative cyclization (OC) of active catalyst with diene and aldehyde, c) a *β*-hydride elimination to give Co(III)-H species, and d) a reductive elimination facilitating the hydride transfer to diene and furnishing the final hydroacylated product. Energetically, we found that the branched and linear diene follow different OC modes yielding disparate regioisomers. The substrate-controlled regioselectivity switching was unveiled to depend on the number and strength of noncovalent interactions (NCIs) between substrates (diene and aldehyde) and catalyst. In addition, the reductive elimination is the enantiocontrolling step for branched diene, whereas, for linear diene, the oxidative cyclization step takes precedence. Chiral induction in the enantiocontrolling step is explained through activation strain analysis, revealing that the preferred enantiomer has a lower activation barrier than its counterpart. The *β*-hydride elimination is identified as turnover determining step of the catalytic cycle, independent of regio- and enantiocontrol. These insights enhance the understanding and predictability of hydroacylation reactions.

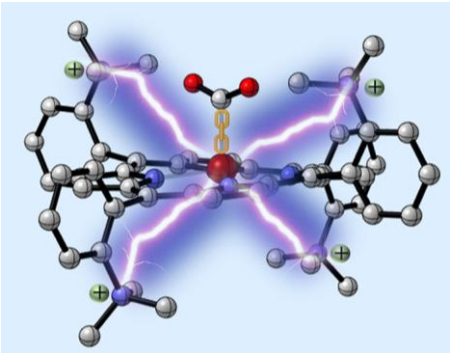
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Electric Fields: The Secret to Breaking CO_2 Conversion Records

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Electrochemical CO_2-to-CO conversion is a critical step in sustainable catalysis, with iron tetraphenylporphyrin (Fe–TPP) derivatives recognised as benchmark catalysts, reaching turnover frequencies (TOFs) up to 10^6 s^{-1} with trimethylammonium (TMA) substitution. However, substituent effects remain unpredictable: sulfonyl groups render the catalyst inactive, while others enhance activity, resulting in over 50 reported analogues without a coherent design principle. Using density functional theory (DFT) and response theory (accounting for electric field effects), we dissect this variability and identify key reactivity drivers. Electronic structure analysis reveals the redox non-innocent behaviour of the TPP ligand, forming species such as $[Fe(II)TPP^{\bullet\bullet}]^{2-}$, stabilised by antiferromagnetic coupling (J = -656 cm^{-1}). The ability of the TPP ligand to transiently hold and transfer electrons during the catalytic cycle significantly boosts catalytic performance. Mechanistic analysis using the energetic-span model for Fe–TPP (**1**), Fe–p–TMA (**2**), and Fe–o–TMA (**3**) yields barriers of 195.5, 184.4, 162.2 kJ/mol, respectively, correctly predicting the experimentally observed trend of **3** > **2** > **1**. Crucially, local electric fields (LEFs), arising from charged substituents, are identified as the dominant factor in tuning reactivity, surpassing traditional steric or inductive considerations. Applying an oriented external electric field of +0.21 V/Å to **1** reproduces the performance of **3**, confirming LEF as a unifying descriptor. Guided by this, we *in silico* design next-generation catalysts with barriers as low as 129.4 kJ/mol, setting a new paradigm for rational electrochemical CO_2 reduction catalysis.



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Theoretical Chemistry Symposium
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Deciphering the mechanism of chain propogation in polymerization via alkene difunctionalisation

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Transition metal-catalyzed alkene difunctionalization involves incorporating different functional groups across an olefin, which is a transpiring and notable reaction utilised to design complex molecular entities.[1] Although this approach has been used in constructing intricate small molecules, its latent potential lies in enabling the design of stereochemically defined polymers with high functional group tolerance.[2] Ni-catalysed alkene difunctionalisation of bromostyrene with arylboronic esters yielding poly [arylene α-(aryl)ethylene]s (PAAEs) is one of the groundbreaking methods for the synthesis of stereo-defined polymers (Figure 1).[3] Interestingly, this new class of polymers exhibited notable physical properties. With the aid of computational methods, we unraveled the mechanism of this polymerization reaction.[4] We were particularly intrigued to study the different modes of chain propogation that leads to the stereospecific functionalized polymers with tailored side chain groups. The regioselectivity and chain propogation feasibility was analysed using AIM, EDA, and NBO analysis.

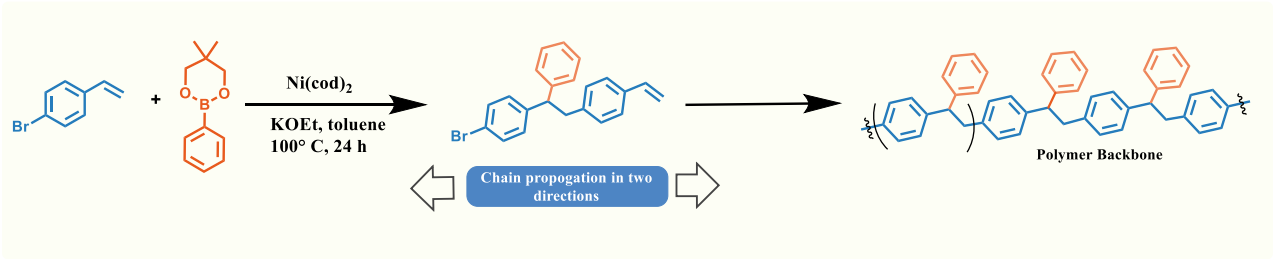


Figure 1 Reaction scheme for the polymerisation of haloarene with boronic ester by 1,2-alkene diarylation

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Theoretical Chemistry Symposium
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CP-Graphyne as a Next-Generation Two-Dimensional Anode Material for Alkali-Ion Batteries: A First-Principles Study"

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CP-graphyne, a novel two-dimensional carbon allotrope, has emerged as a promising anode material for next-generation rechargeable batteries owing to its unique topology, high electrical conductivity, and tunable ion adsorption properties.[1]In this study, the ion storage capability, open-circuit voltage (OCV), and diffusion behavior of Li, Na, and K atoms intercalated into CP-graphyne were systematically examined using first-principles calculations. The adsorption energy analysis confirmed that all three alkali metals exhibit favorable binding with the CP-graphyne surface, suggesting strong thermodynamic stability upon intercalation. The calculated OCV profiles showed a gradual decrease with increasing ion concentration, indicating efficient ion insertion and enhanced electronic conductivity in the fully loaded states. The ion migration behavior, explored through the nudged elastic band (NEB) method, revealed that all the alkali ions can diffuse effectively across the surface, with potassium exhibiting relatively superior mobility. Furthermore, *ab initio* molecular dynamics simulations demonstrated that the fully intercalated CP-graphyne structure remains thermally stable under ambient conditions without noticeable structural deformation, confirming its mechanical robustness during repeated ion insertion and extraction. Overall, these findings highlight the excellent adsorption affinity, favorable voltage response, fast diffusion kinetics, and strong thermal stability of CP-graphyne, establishing it as a highly potential anode material for Li-, Na-, and K-ion battery systems.

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Beyond Red: Uncovering New NIR-TADF Emitters One Bit at a Time

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Near-infrared (NIR) thermally activated delayed fluorescence (TADF) materials are emerging as critical components in technologies ranging from organic light-emitting diodes to bioimaging and photodynamic therapy. Despite their promise, the rational design of efficient NIR-TADF emitters remains hindered due to limited diversity in known acceptor motifs and the inherent energy-gap law, favoring non-radiative pathways at lower energies. In this work, we introduce a machine learning (ML)-guided strategy to accelerate the discovery of novel NIR-TADF candidates by leveraging the rich structural diversity of non-fullerene acceptors (NFAs). Through interpretable fingerprint-based modeling, we identify substructures responsible for red-shifted absorption and strategically recombine them with TADF donor motifs to generate a diverse molecular library. Our method integrates quantum-chemical methods with data-driven feature analysis to pinpoint fragment-level design rules that promote long-wavelength emission. This framework not only offers a sustainable and cost-effective path for navigating unexplored regions of chemical space, but also paves the way for data-efficient inverse design of next generation NIR-TADF emitters.

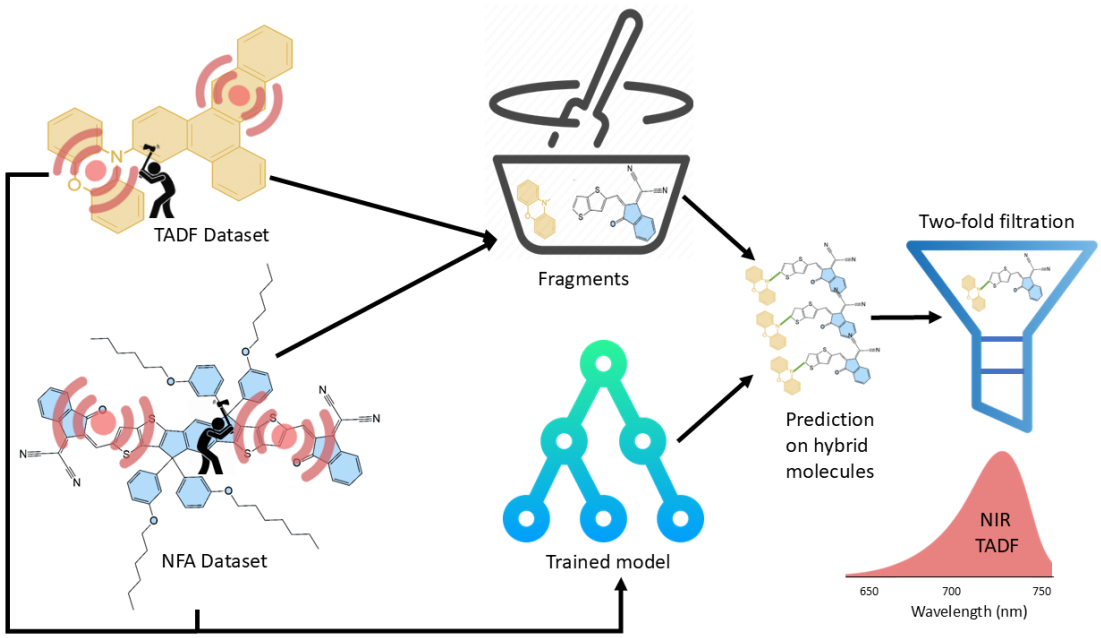


Figure 1 A schematic representation of the workflow implemented in this study.

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Conformational Landscape of Semi-flexible Polyampholytes

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Abstract: Intrinsically disordered proteins (IDPs) play central roles in biology, including cell signaling, regulation, and biomolecular condensation. Unlike folded proteins, they lack stable structures and instead explore a wide conformational space. A useful way to model and understand their behavior is through polyampholytes—polymers carrying both positive and negative charges—since IDPs often contain mixed-charge sequences. Studying polyampholytes provides physical insight into how sequence features shape IDP conformations and functions. While most work has focused on the influence of solvent or electrostatic strength, less attention has been given to the role of chain stiffness. Many biological polymers, including IDP s bound to partners or confined in crowded environments, are not fully flexible but instead exhibit semi-flexible behavior. This raises the question of how bending rigidity interacts with charge sequence patterning to determine structure. Using coarse-grained molecular dynamics simulations, we explore the conformational and dynamical properties of semi-flexible polyampholytes under fixed electrostatic conditions. We find that semiflexibility couples nontrivially with charge organization. Furthermore, mean-squared displacement (MSD) analysis reveals distinct dynamical signatures between these states, showing how stiffness and sequence jointly regulate both structure and dynamics. Our results provide a framework for understanding IDP preferences from a polymer physics point of view and for designing programmable polymers with tunable morphologies and mobility.

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IN SILICO DESIGN OF JAK3 INHIBITORS: DFT ANALYSIS, MOLECULAR DOCKING AND ADMET PREDICTION WITH DECERNOTINIB AS A LEAD MOLECULE

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Decernotinib is found to be in the developing stage for the treatment of Rheumatoid arthritis by inhibiting its corresponding protein PDB ID(5TTV). To explore the structure and property relationship, we have designed totally eight α,β-unsaturated ketone compounds substituted derivatives.The geometrical features of all the molecules have been addressed from Density Functional Theory calculations. Chemical reactivity descriptor analysis was carried out to understand various reactivity parameters. The drug-likeness properties were estimated by a detailed ADMET.The binding ability and the mode of binding of these derivatives into the protein structure are obtained from molecular docking studies and the calculations show greater binding ability for the designed inhibitors compared to that of the experimentally reported lead molecule. Overall, the present work proves to offers new insights and guidelines for synthetic chemists to develop new drugs using α,β unsaturated ketone compounds substituted Decernotinib in the treatment of Rheumatoid arthritis.

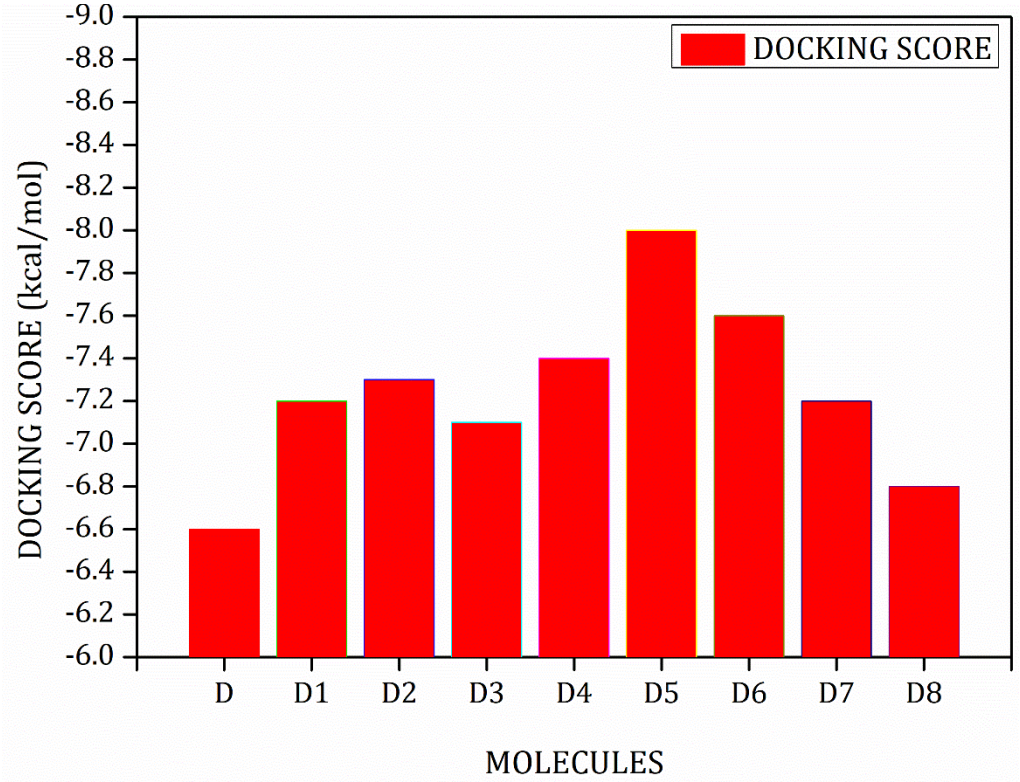


Figure : Graphical representation showing docking score of the lead molecule and its derivatives

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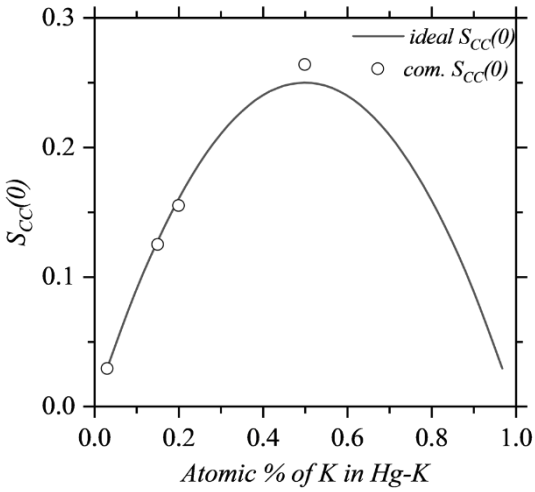
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Theoretical Studies on Structure, Correlations and Associated properties of Binary Liquid Hg–K Alloys Through Liquid State Theories

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Structure and correlations have been studies in binary liquid Hg–K alloys using the perturbation theories for partially ordered systems by considering them as square-well liquids. The structure factor S(k) was computed using their generated pair-potential functions and subsequently employed to evaluate the radial distribution functions and the associated properties such as the long-wavelength limit of structure factor $S(0)$, Bhatiya-Thronton concentration-concentration correlation function in zero momentum vector, i.e. $S_{CC}(0)$, coordination number, diffusion coefficient, and isothermal compressibilities at different compositions and temperatures. The results were compared with the available experimental data and found in good agreement.

Table 1 Theoretical and experimental principal peak heights and positions of structure factors of Hg-K alloys.



Atomic % of K in Hg-K alloys	Theoretical values		Experimental values	
	k (Å^{-1})	S (k)	k (Å^{-1})	S (k)
3	2.43	2.53	2.43	2.64
15	2.39	2.75	2.43	2.62
20	2.35	2.61	2.43	2.57
50	2.23	2.39	2.33	2.35

Figure 1 $[S_{cc}(0)]_{Ideal}$ and $[S_{cc}(0)]_{Computed}$, plotted against the atomic percentage of potassium in binary Hg-K liquid alloys.

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Implicating the Role of Enhanced Oxyl Attribute in Facil- itating Exceptional C-H Activation by a [$Co^{III,IV}_2(\mu\text{-}O)_2$] Diamond-Core Complex: A Theoretical Perspective

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C-H activation is a key biochemical process often facilitated by heme and nonheme enzymes through high-valent metal-oxo species. Among these, nonheme dinuclear iron-dependent enzyme, soluble methane monooxygenase (sMMO), stands out for its ability to activate strong C-H bonds via a diiron(IV) intermediate[1]. Our study focuses on a cobalt diamond core complex [$Co^{III,IV}_2(\mu\text{-}O)_2$] supported by a tris(2-pyridylmethyl)amine(TPA) ligand, which has been experimentally proven to have a remarkably high rate constant for C-H bond activation in 9,10-dihydroanthracene(DHA), surpassing analogous first-row transition metal complexes, including the well-established diiron systems[2]. Employing Broken Symmetry Density Functional Theory (BS-DFT) and Complete Active Space Self-Consistent Field (CASSCF) methods, we have theoretically investigated the mechanistic pathways through the prism of multi-state reactivity and unearthed the electronic factors driving such C-H activation process. Comparative barrier analyses between cobalt and iron diamond core complexes further reveal the distinctive advantages of the cobalt system in understanding metal-oxo mediated hydrogen abstraction

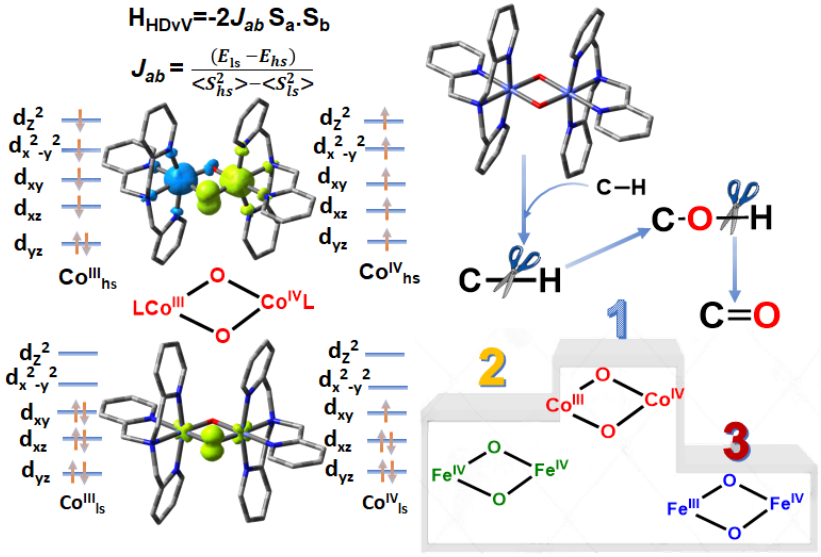


Figure1: Schematic representation of the work

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Correlation of Structure with Acoustic and Transport Properties in Si-Ni Alloys at Varying Temperatures and Compositions.

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Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, U.P., 221005, India, Corresponding Author Email address: venkateshbhu@yahoo.co.in;

Simple models cannot adequately describe the structural and their related properties of liquid Si-Ni alloys because they are extremely complicated metallic systems. The repulsion and excluded-volume effects of the ions are initially studied using the hard-sphere model as a reference. Then, to adjust for attractive interactions, a square-well potential is introduced. Total structure factors are obtained by combining partial structure factors for several atomic species using the Ashcroft–Langreth technique. The local arrangement of atoms is described by the radial distribution functions $g(r)$, which are obtained using Fourier inversion. These are used to evaluate diffusion coefficients and coordination numbers, which establish a connection between atomic mobility and structural order. Structure factors give access to bulk characteristics in the long-wavelength limit: thermodynamic relations are used to determine the velocity of sound, and compressibility is derived from the zero-wavevector limit.

Table 1. Computed and experimental values of compressibilities, long wave limit values of total structure factors, and velocities of sound.

Atomic % of Si in Si-Ni melts	Temp. (K)	β_T $(10^{-11}\ Pa^{-1})$		S(0) = $\rho k_B T \beta_T$ (10^{-2})		Velocity of sound (10^3 m/sec)	
		Theo.	Expt.	Theo.	Expt.	Theo.	Expt.
10	1673	6.33	5.71	1.511	1.3722	1.45	1.37
25	1673	6.39	5.72	1.727	1.5456	1.54	1.40
40	1523	8.70	9.40	2.195	2.3702	1.62	1.41
50	1323	10.60	11.70	2.255	2.5033	1.67	1.41

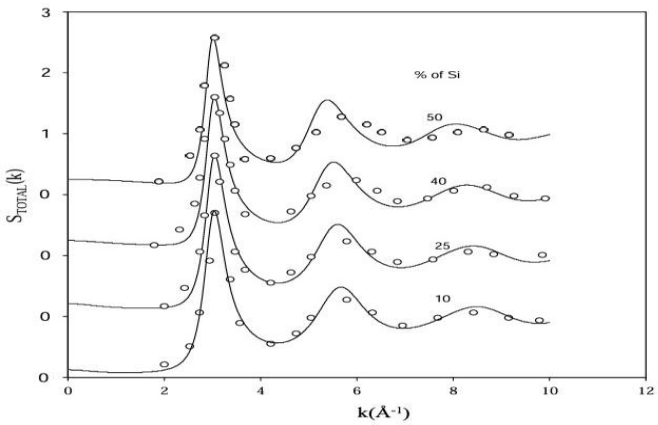


Figure 1 Total structure factors $S_{TOTAL}(k)$ versus k at 10, 25, 40, and 50 percent Silicon.

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Graph Neural Network–Driven Yield Prediction in Transition Metal–Catalyzed Cross-Coupling Reactions

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Machine learning (ML) is transforming diverse scientific disciplines, including chemistry. Among various ML approaches, graph neural networks (GNNs) have emerged as powerful frameworks for modeling complex relationships by representing data as graphs. One rapidly growing application of GNNs is in predicting chemical reaction yields. However, effectively managing heterogeneous datasets remains a significant challenge. In this study, we employed diverse datasets encompassing a range of transition metal-catalyzed cross-coupling reactions, including Suzuki, Sonogashira, Cadiot–Chodkiewicz, Ullmann-type, and Buchwald–Hartwig couplings. To predict reaction yields, we implemented and compared multiple GNN architectures—message passing neural networks (MPNN), residual graph convolutional networks (ResGCN), graph sample and aggregate (GraphSAGE), graph attention networks (GAT and GATv2), graph convolutional networks (GCN), and graph isomorphism networks (GIN). Among these, the MPNN model achieved the best performance, attaining an R^2 value of 0.75. When used for test data containing 90% Pd catalysts, the MPNN model achieved a predictive accuracy with an R^2 of 0.98 in chemical yield prediction. reactions. This work contributes to the application of machine learning in catalysis, providing valuable insights for optimizing catalytic reactions and contributing to innovations in sustainable chemistry and organic synthesis.

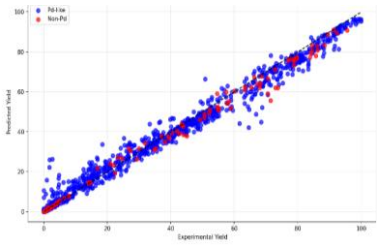


Figure1 : Scatter

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The curious case of co-planarity in di-nuclear triel complexes: a density functional investigation

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Density functional investigation of intramolecular triel (Tr) bonding present in di-nuclear aryl complexes of group 13 elements having general formula $[(Tr)Me_2\ (2,6\text{-}(X)_2C_6H_3O)]_2$ (Tr = B, Al, Ga, In & Tl and X = OMe, OEt, OH, OPh, NH_2, SH, Cl, F) has been performed. Conclusive evidence of the concurrent two σ-hole interaction has been provided by analysis of the Tr bond length, interaction energy (ΔE), second order perturbation energy (E^2), charge transfer (Δq), quantum theory of atom in molecules (QTAIM) and noncovalent interaction (NCI) plots for 12 complexes. The Tr bond length in the optimized geometry varies from 2.49 to 2.89 Å in Al complexes and 2.66 to 2.83 Å in other group 13 element complexes at the PBE0-D3 functional. The interaction energy calculation reveals that the co-planar structure of complexes containing Al are more stable than their rotamers by 8–15 kcal/mol , whereas the di-nuclear complexes of other group 13 complexes orient in a non-planar pocket structure. This loss of co planarity reveals the fact that its presence relies on the Tr atom, not the intramolecular Tr bonding, which has a striking impact on the crystal engineering of di-nuclear complexes of Group 13.

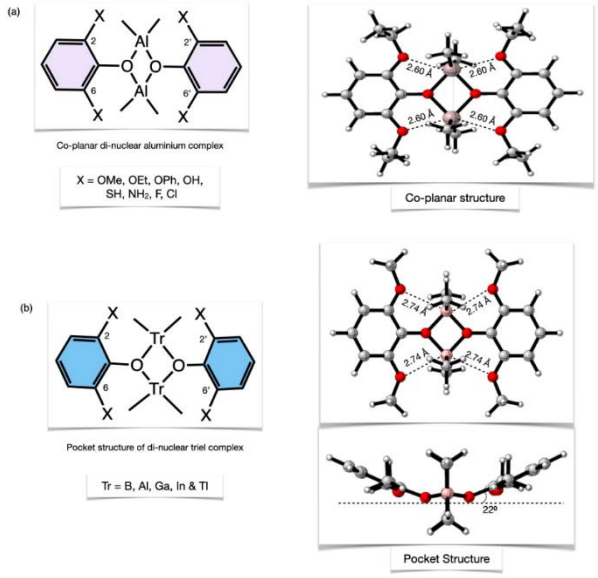


Figure 1 Caption

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In Silico Studies of Spin crossover systems on surfaces

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The use of molecules or molecular assembly for the use of information processing presents one of the best possible objectives for chemists so that they can use a synthetically modified chemical to be found in industrial applications. Although it seems to be a long-term plan, some key aspects have already been reported. Among those features, molecular bistability is one of the fundamental underlying concepts that seems to be helpful for us. Molecular bistability can be defined as if the molecular system is stable in two different states and in a given range of perturbation.[1] Among these two states, one will be the stable state or ground state, and the other will be the meta-stable state. One such example of molecular bistability is named Spin Crossover (SCO). The SCO complexes are generally found to be transition metal complexes from d^4-d^7 metal ions. The SCO complexes are very useful in data storage and sensing devices. But for any of the devices to work, the complex has to be grafted on top of a surface that can be metallic or non-metallic.[2] Due to the very low energy barrier between the states of SCO, the choice of surface matters a lot when designing a device. Hence, we want to study the binding of the SCO complex with the surface and how the surface reacts to a complex to understand the effect of the surface on an SCO complex by doing computational study. In this case, the complex Fe [HB(3,5-$(CH_3)_2$pz)$_3$]$_2$ (Fe-pz) has been chosen as it was proved to be stable on the Au (111) surface, which is very rare because the Au surface is the most reactive surface to study and it very easily destroys many SCO complexes known prior.[3] By modeling the complex on the Au(111) surface and in the presence of a Ferromagnetic Co surface, it was possible to study the system to understand better how the surface reacts to the SCO systems.

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Correlation of Structure with Acoustic and Transport Properties in Si-Ni Alloys at Varying Temperatures and Compositions.

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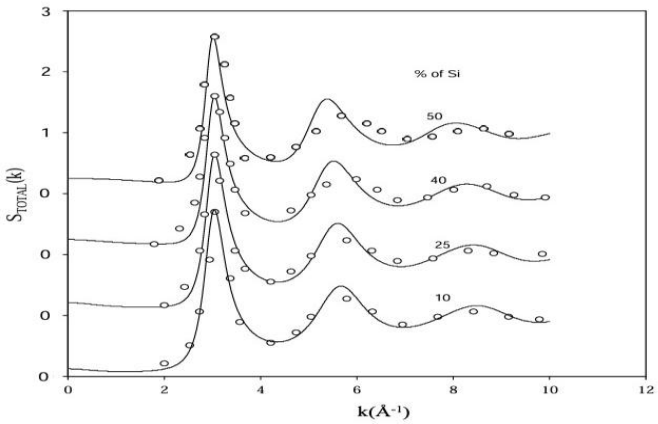


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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

A Comparative Study on the Photo and Thermal Reaction Pathways of Two Different Types of Imidazole N-oxide systems

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The acyclic and cyclic N-oxides are well-known for their pharmacological and biological importance. These compounds are used in several drugs related to age-related diseases, stroke treatment, chemo prevention of cancer and so on. Many compounds of this class are highly significant in biological fields due to their spin-trapping ability through which they can bind short lived radicals. The EPR signals or the immuno-spin trapping studies are used to detect these transient radicals. In the last one and half decade, our computational group have revealed the unexplored photochemistry of several acyclic and cyclic N-oxide systems. Among the latter type of systems, pyrroline N-oxides like DMPO [1,2], 2H-imidazole 1-oxides like TMIO, DMPIO [3] and 2H-imidazole 1,3-dioxides had been reported by Chattopadhyay and co-workers. Most of these systems are well-known spin-trapping agents. A new addition in this list is our recent studies on 4H-imidazole-N-oxides [4]. We have successfully captured their photo-isomerization pathways (4H-imidazole 3-oxides→oxazirdine and 4H-imidazole 1,3-dioxide → *trans,cis*-dioxaziridines) along with the thermal reverse isomerization of the photoproducts. The computed results have justified the experimental observations reported on these systems and the study has established proper mechanisms behind the mentioned processes. Presence of conical intersection channels involving the low-lying singlet states (S_0, S_1, S_2 and S_3) has been identified along the photo-isomerization pathways, similar to the analogous 2H-imidazole-N-oxide systems. The reverse thermal conversion oxaziridine→4H-imidazole 3-oxide is found to depend on the nature of the substituent present at the 2-position. In comparison to methyl group, the presence of phenyl ring at this position, especially with electron-donating groups, is found to make this conversion faster. Additionally, these studies also highlight other reported observations like the faster reverse thermal conversion of 4H-imidazole 3-oxides in comparison to that of the 2H-imidazole 1-oxide systems. Another contrasting feature explained through our work is the better tendency of 4H-imidazole N-oxides to form the radical cations under oxidation. Currently our group is involved in similar studies on other types of imidazole N-oxide systems.

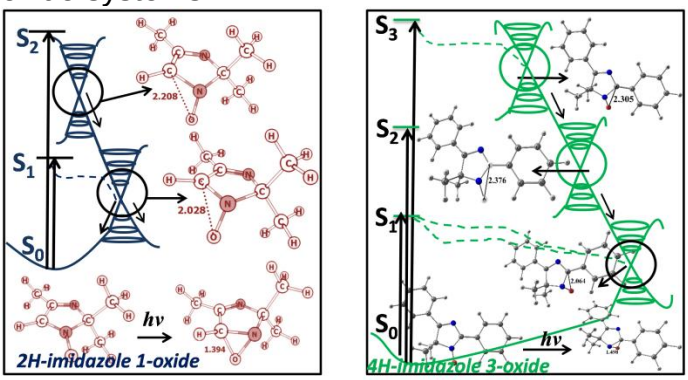


Figure 1. Schematic representations of the photo-isomerization pathways of the two imidazole N-oxide systems

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Modulating Quantum Interference in Coronene-Based Molecular Junctions via Isoelectronic B-N Substitution at Selective Positions and Patterns

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In silicon-based semiconductors, doping a small amount of trivalent or pentavalent elements modulates conductance substantially by increasing the concentration of charge carriers. However, in single-molecule junctions (SMJ), functional substitution and doping have only a modest impact on conductance. Significant conductance modulation can be achieved by harnessing quantum interference (QI) effect, which requires major changes in the structural topology, charge state or redox reactions.[1] This raises a key question: Can chemical substitution or doping alone be strong enough to switch QI behaviour and considerably modulate conductance? To address this, we investigated the effect of isoelectronic B-N substitution on QI in synthetically relevant coronene-based SMJs by selectively replacing C=C bonds with B-N pairs at various positions and patterns, employing a combination of density functional theory and non-equilibrium Green's function methods. Our calculations reveal that position- and pattern-dependent B-N substitutions can strongly perturb the molecular orbital symmetry, phases, and energies in such a way that switch QI characteristics and finally modulate conductance remarkably. The QI features remain unchanged even at finite bias, and align well with the orbital phase analysis and local current circulation pathways. This work demonstrates a novel design strategy to harness QI effect in polyaromatic hydrocarbon-based SMJs.[2]

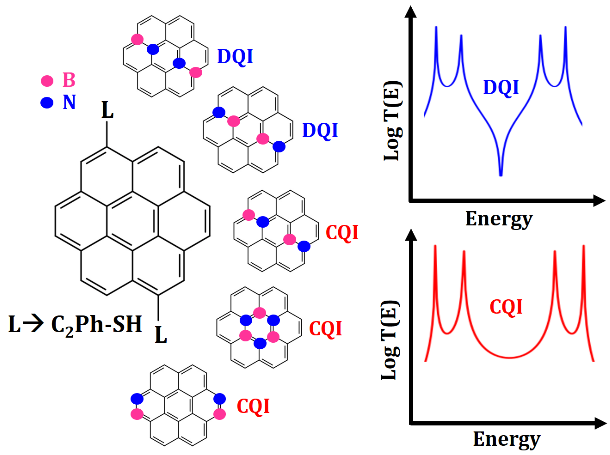


Figure 1 Schematic representation of quantum interference in BN-substituted coronene-based molecular junctions

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Breaking Azeotropes: The Role of an Entrainers in Mixture Separation

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Separation of azeotropic mixtures with conventional fractional distillation technique remains a persistent challenge in the chemical and pharmaceutical industries. To overcome this challenge, entrainers are widely used in azeotropic separation. An entrainer is a component that helps to break an azeotrope, enabling easier separation of the original components during distillation. Selecting a suitable entrainers for the separation of azeotropic mixture is a key step. The traditional method for solving this problem is experimentation, which is time consuming and expansive. Therefore, understanding the role of entrainers in azeotrope separation is of critical importance. Molecular Dynamics (MD) simulation provides an effective approach to investigate these things. This study investigates the ethanol–water azeotrope using 1-ethyl-3-methylimidazolium chloride ([EMIM]Cl) ionic liquid and benzene as entrainers. In the presence of entrainers, we observed significant changes in the diffusion behavior of both ethanol and water, which can be attributed to alterations in the hydrogen bonding between the components. The results indicate that the ionic liquid interacts more strongly with both components and reduces the extent of hydrogen bonding between the species more effectively than benzene. The diffusion coefficient of water decreases more significantly than ethanol. The findings of this study offer molecular-level insights demonstrating the superior performance of ionic liquids compared to conventional entrainers like benzene.

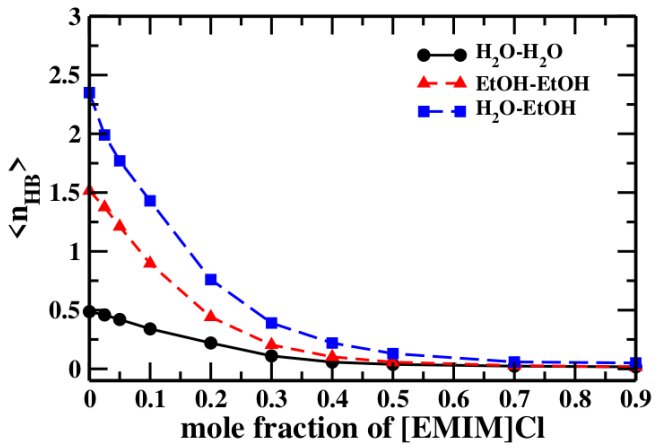


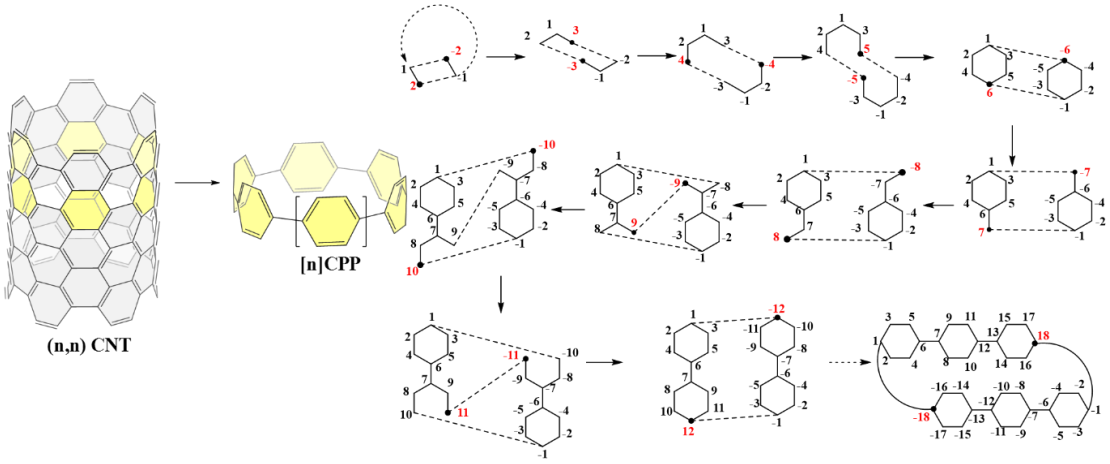
Fig. Number of hydrogen bonds between different components.

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Low-lying excited electronic states of Cycloparaphenylene and Cyclacene: A symmetrized Density Matrix Renormalization group study with periodic boundary condition

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Low-lying excitations for one-dimensional and quasi one-dimensional correlated systems can be studied numerically with the Symmertized Density Matrix Renormalization Group (SDMRG) method[1]. On the other hand, molecules in non-one-dimensional systems can be built in this scheme so that the entanglement between their two constituents remains relatively constant and controllably low[2]. The sites introduced at each stage are carefully chosen to achieve this. Because the density matrix eigenvalues decrease more quickly with open boundary condition (OBC) than with periodic boundary condition (PBC), which result in more accurate convergence, OBC is commonly used in SDMRG calculations. There are two ways to improve the accuracy of a PBC system in DMRG calculation: increasing the number of states cutoff basis retained to characterize the system and performing one or more iterations of the finite-size algorithm[3]. The correlated excited-state spectra of [6]cycloparaphenylene and [n]cyclacene are studied using this approach in conjunction with the Pariser-Parr-Pople (PPP) model, which takes into account long-range electronic correlations. Additionally, we have examined the bond orders and spin densities in triplet states of these PBC systems.



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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Interactions of alkali metal atoms and electrolytes with redox-active covalent organic framework-based organic electrodes

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The redox-active covalent organic frameworks (COFs) have emerged as promising electrodes for alkali metal ion batteries. In this work, we investigate the structural and dynamic properties of a triquinoxalinylene-benzoquinone[1,2] (TQBQ) COF (Figure 1) as a potential electrode for alkali metal ion batteries. We employed density functional theory (DFT)-based calculations to study the nature of interactions between alkali metal atoms and the TQBQ-COF. First, different configurations of the COF-scaffold were modeled to identify the stable structure, which was then used for further calculations. The key electrochemical parameters, such as average adsorption energy and average voltage, were calculated. The DFT results highlighted the structural stability and reversibility of the TQBQ-COF electrode. We then extend our study on the interaction of electrolytes with the TQBQ-COF using ab initio molecular dynamics (AIMD) simulations. Our results establish a strong computational foundation for modeling realistic electrode-electrolyte interfaces, providing molecular-level insights that are critical for designing high-performance COF-based organic electrodes for alkali metal ion batteries.

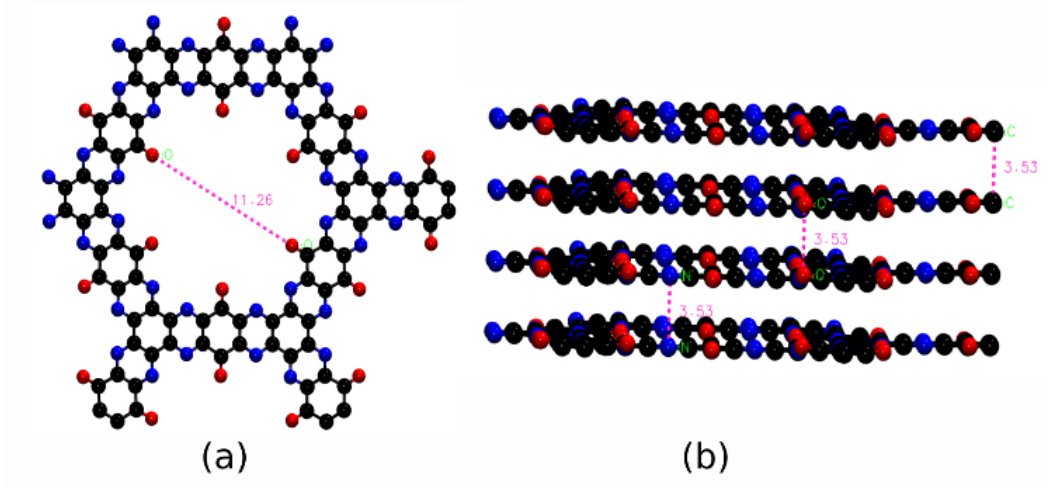


Figure1. The DFT-optimized structure (a-top view and b-side view) of TQBQ-COF in a hexagonal lattice. The TQBQ-COF model consists of four atomic layers. The pore diameter and the optimized inter-layer distance are highlighted in a pink coloured dashed line. Atoms color: C-black, N-blue, and O-red.

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Ni(III)/Fe(III) Ground State: Key to [NiFe]-Hydrogenase Oxygen Tolerance

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The critical oxygen tolerance observed in certain [NiFe] hydrogenase enzymes is essential for developing effective bio-inspired hydrogen catalysts.[1,2] The fully oxidized state of the *Hydrogenophilus thermoluteolus* SH (Ht SH) hydrogenase features an unusual NiFe active site coordinated by terminal glutamate and three bridging cysteine residues, a structure detailed by X-ray crystallography.[3] This architecture previously led to an initial assignment of an unprecedented high-valent Ni(IV)/Fe(II) closed-shell singlet (CS, S=0) in the oxidized enzyme.[4]

To definitively determine the electronic ground state, we utilized large Quantum Mechanical (QM) cluster models (>300 atoms) and hybrid QM/Molecular Mechanics (QM/MM) calculations (392 atoms). Our analysis consistently demonstrates that the broken-symmetry (BS) Ni(III)/Fe(III) state is the energetically favored electronic ground state over the previously proposed closed-shell assignment.[4,5] This BS state is an open-shell singlet (S=0) characterized by antiferromagnetically coupled metal centers.[5,6]

Furthermore, detailed orbital analysis revealed an unusual three-center two-electron (3C-2e$^-$) bond involving the nickel center and coordinating sulfur atoms, which substantially enhances the electronic stability of this open-shell ground state.[5] We conclude that the stabilization provided by this Ni(III)/Fe(III) electronic configuration serves as a molecular safeguard against irreversible oxidative deactivation, underpinning the enzyme's resilience and offering key insights for metalloenzyme redox adaptation.[5,6]

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Magnesium Regulates RNA Ring Dynamics and Folding in Subgenomic Flaviviral RNA

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Mosquito-borne flaviviruses, including dengue, Zika, and yellow fever, generate a large number of subgenomic flaviviral RNAs (sfRNAs) during infection in human cell. A conserved segment of this RNA, named as xrRNA1, adopts a multi-pseudoknot (PK) architecture that blocks degradation of the viral RNA by the host exonuclease XRN1. We investigate how this long-range RNA PK folds in the presence of a mixed ion environment, specifically in a mixture of monovalent (K^+) and divalent (Mg^{2+}) salts at physiological concentrations. Here, we combined extensive explicit-solvent molecular dynamics (MD) simulations with an all-atom structure-based modeling to investigate the folding mechanism of xrRNA1. Explicit MD simulation studies allowed precise mapping of RNA–Mg^{2+} interactions, distinguishing inner-sphere (chelated) from outer-sphere coordination. To capture large-scale conformational transitions, we employed an implicit–explicit hybrid ion model within an all-atom structure-based RNA framework, probing folding dynamics both in the absence and presence of physiological Mg^{2+}. Our simulations reveal a dynamic equilibrium between the ring-open and ring-closed conformational states, governed by long-range PK interactions. Free-energy calculations demonstrate that Mg^{2+} shifts this equilibrium toward the ring-closed state. Ion-mediated contact probability maps further highlight a critical Mg^{2+} bridge between G50 and A33 residues, which stabilizes the PK and promotes ring closure. Together, these results define Mg^{2+} as a key determinant of xrRNA1 folding, directly stabilizing long-range PK interactions that underlie XRN1 resistance. This work provides molecular-level insights into the ion-dependent folding pathways of flaviviral xrRNAs and their role in enhancing viral RNA stability.

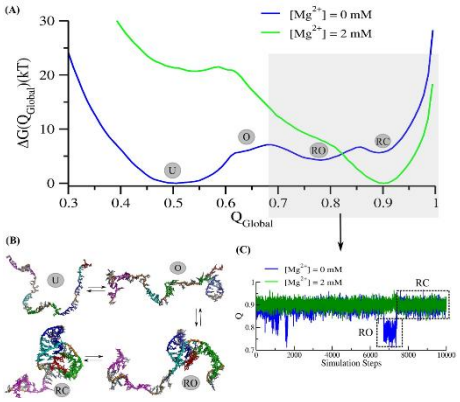


Figure 1. (A) The folding free energy profile reveals four distinct minima, separated by energy barriers. These minima correspond to four stable states. (B) The representative structures of the four states identified in the free energy profile are: (i) Unfolded state (U), (ii) Open state (O), (iii) Ring-opened state (RO), and (iv) Ring-closed state (RC). (C) Evolution of the fraction of native contacts (Q) from equilibrium simulations specifies the transition between RO and RC states.

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Unveiling the activity and selectivity of single metal atom supported on AlN monolayer for electrochemical conversion of NO to NH_3: A DFT study

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Electrochemical nitric oxide reduction reaction (NORR) is a promising alternative method to capture and utilize NO, emitted due to the massive acceleration of the nitrogen cycle resulting from various human activities[1]. In this study, the NORR catalytic performance of a series of single transition metal (M) atoms anchored on two-dimensional aluminium nitride (AlN) monolayer, *i.e.*, M@AlN (named single-atom catalyst (SAC)), is performed by using spin-polarised density functional theory (DFT) [2] calculations including dispersion corrections [3]. The stability of all M@AlN monolayers, NO adsorption configurations, electrochemical pathways involving proton-electron pair ($H^+ + e^-$) transfer, and the corresponding free energies (using computational hydrogen electrode (CHE) approximation)[4] are computed. Among our modelled SACs, Pd@AlN is found to be the most promising one, which efficiently converts adsorbed NO molecule to NH_3 with a lowest limiting potential of -0.22 V. Further, it significantly suppresses the main competitive hydrogen evolution reaction (HER), resulting in high Faradaic efficiency for NH_3 production. This work may shed light on the design and exploration of new catalysts for NO reduction to NH_3 and provide a valuable reference for further experimental analysis.

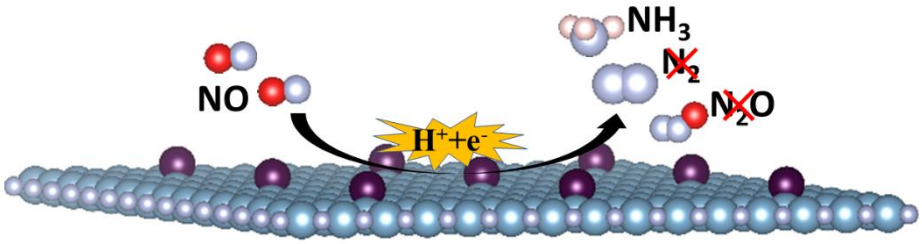


Figure 1: Sustainable development for the green environment - electrochemical conversion of toxic NO pollutant to value-added NH_3 through single-atom catalyst strategy

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Unravelling the Prebiotic Origins of Simplest α-Ketoacids in Cometary Ices: An ab initio Nano Reactor (AINR) Approach

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The metabolism-first approach to prebiotic chemistry centers on key metabolic cycles like the tricarboxylic acid (TCA) and reverse-TCA (r-TCA) cycles. Central to these, as well as the proposed hydroketoglutarate-malonate cycle, are the two simplest α-ketoacids: glyoxylic acid (Gly) and pyruvic acid (Pyr). Broader analyses of metabolic pathways suggest these two compounds serve as critical biochemical junctions. Therefore, understanding the prebiotic origin of these foundational α-ketoacids is crucial. This study utilizes *ab initio* nanoreactor (AINR) and density functional theory (DFT) calculations to explore a plausible extraterrestrial synthesis route. We investigate how the shock compression of common interstellar ice components- embedded within comets entering Earth's early atmosphere- could have generated glyoxylic and pyruvic acids, thereby providing the essential α-ketoacids required for the inception of metabolic cycles.[1]

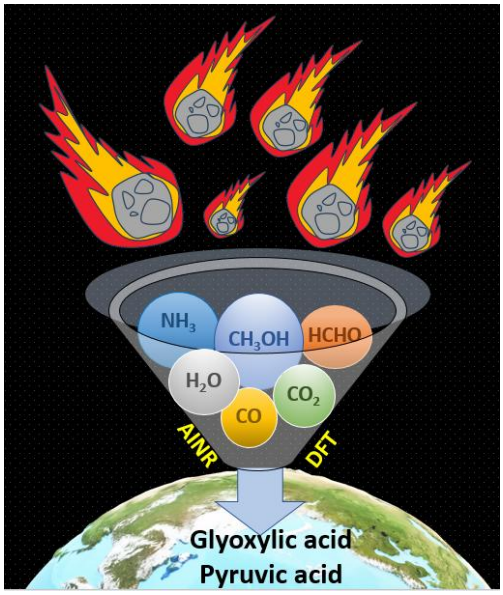


Figure 1: The schematic representation detailing the extraterrestrial origin of the simplest α-ketoacids, as revealed by simulating the impact shock compression of interstellar ice components trapped inside a comet

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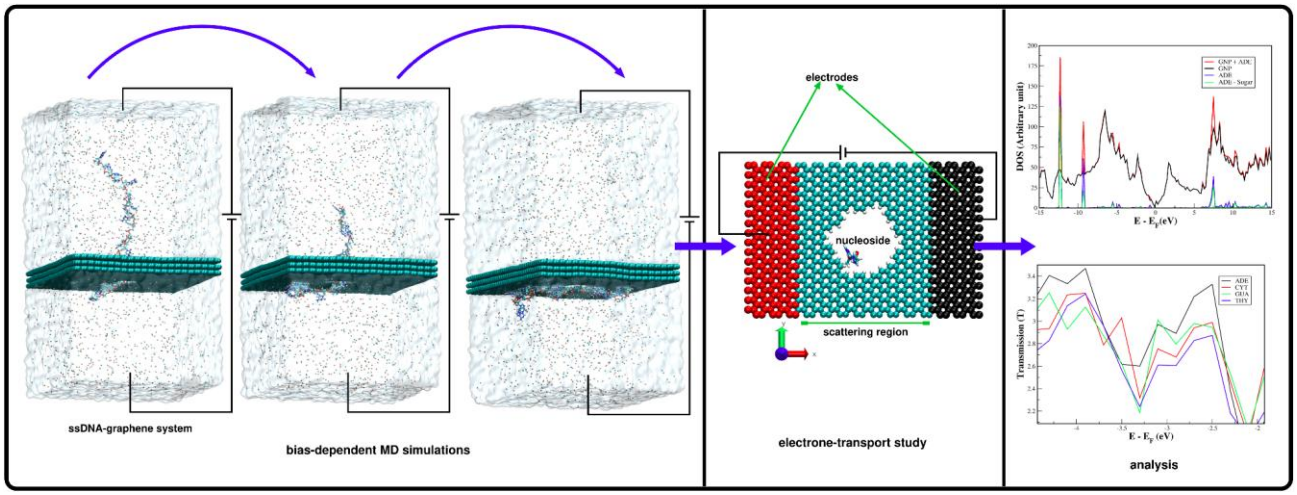
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DNA Dynamics in Graphene Nanopore: Insights and Sequencing Challenges

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Understanding nucleic acid sequences has always been a crucial aspect of genomics[1]. DNA sequencing has broad applications across three major domains: (i) biological and medical sciences, (ii) administrative fields, and (iii) development of microelectronic devices[1,2]. Graphene has recently gained significant attention as a promising solid-state nanopore material[3,4]. According to existing literature, most established nanopore-based sequencing methods have used protein-based pore embedded in biological membranes. However, these biological systems are fragile, sensitive to external perturbation and difficult to handle[5]. As an alternative, we used graphene-based nanopore to investigate the DNA sequencing efficiency through atomistic resolution.

In this work, we designed a sensing system composed of tri-layer graphene with a centrally located nanopore, through which a 20-mer heteromeric DNA strand was placed transversely. Non-equilibrium molecular dynamics (MD) simulations were carried out using Drude polarizable force field[6]. We studied the directional electrokinetic movement of DNA through the nanopore. From the classical trajectories, we analysed the nucleobase-nanopore interactions. To assess the feasibility of nanopore based sequencing we performed classical ionic-current analysis and zero-bias transmission spectral study. This multiscale approach, combining MD simulations and electron-transport study, offers a comprehensive understanding of the sensing mechanism and highlights both its potential and limitations.



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Developing anisotropic potential to model non-covalent interactions in non-spherical fullerenes

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Since the discovery of fullerenes in 1985[1], researchers have primarily focused on the more stable class of fullerenes, such as C_{60} and C_{70}. However, non-spherical fullerenes remain less explored due to their instability and incompatible geometries. To fully harness their potential, it is essential to understand how these fullerenes interact with one another. Analytical potentials become necessary to characterize non-covalent interactions in fullerene aggregates as ab initio approaches are computationally expensive for such large systems. The first continuum-modeling based analytical potential for C_{60} was proposed by Girifalco[2] in 1992, and it is widely used till date to model C_{60} clusters. Since then, various models such as the Pacheco-Prates-Ramalho (PPR)[3] potential have been proposed. Nonetheless, these models fail when addressing interactions in non-spherical fullerenes.

In this study, we developed a new analytical approach specifically tailored for ellipsoidal fullerenes such as C_{24}, C_{30}, C_{36}, and C_{40}. Unlike C_{60}, which is spherical, these molecules show clear anisotropy due to their ellipsoidal shapes. This leads to interaction patterns that existing spherical models cannot capture. Our approach goes beyond the limitations of Girifalco and similar isotropic potentials by including anisotropic factors that reflect the geometric differences of these structures. We systematically validated the new potential against high-level ab initio calculations, specifically ωB97X-D3BJ/def2-TZVPPD, which acts as a reliable benchmark. We also compared the energetics obtained using the potential to those obtained using established models such as the improved Lennard-Jones[4] potential and the PPR[3] potential to establish improvements in accuracy and transferability.

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Model Potentials for Electron Attachment to Liquid Water

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Electron attachment to liquid water, a central process in radiation chemistry, electrochemistry, and interfacial charge transfer, is governed by the position of the conduction band minimum (CBM).[1,2] Accurately determining the CBM remains a significant challenge due to the complex interplay of electronic correlation, nuclear quantum effects, and structural fluctuations, as well as the prohibitive computational cost of many-body ab-initio methods.[3] This work introduces an efficient and accurate model potential, scaled static Coulomb-hole screened-exchange (α-st-COHSEX), rooted in many-body perturbation theory. This model combines exact exchange and a static screened Coulomb interaction term[4,5] which is scaled by a parameter obtained from parameterization against high-level methods for small clusters. This approach effectively incorporates many-body screening effects while retaining computational efficiency suitable for large-scale molecular and periodic simulations. We use α-st-COHSEX to model CBM of bulk-water and water-vacuum interface and discuss our results against existing experimental and theoretical methods.

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Molecular Insights into Solvation Structures and Ion Transport Mechanisms in Glyme-Based Electrolytes for Potassium-Ion Batteries

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The growing demand for safer and more efficient energy storage devices has led researchers to investigate alternatives to Li-ion batteries. Potassium (K) emerged as a promising candidate for next-generation energy storage devices due to its small stokes radius, high negative redox potential, and, most importantly, it does not form an alloy with aluminum.

Despite many advantages, the high reactivity of potassium shows significant challenges, including uncontrolled side reactions and unstable solid electrolyte interphase (SEI) at interfaces, resulting in low cycle life and capacity fading. To encounter these issues, researchers investigate different combinations of salts, solvents and additives in electrolytes. The solvation structure and dynamics[1-3] of the electrolyte plays a crucial role in determining the performance and smooth functioning of the battery.

We employ a combination of MD simulations and DFT to gain deeper insights into the solvation structures and electrochemical stability windows of glyme-based electrolytes. In this study, we systematically investigate the effect of glyme chain length on solvation environments and their influence on electrolyte properties. A comprehensive structural and dynamical analyses was carried out to elucidate the behavior of different electrolyte compositions. Statistical evaluation of solvation structures provided a clear understanding of the underlying ion transport mechanisms operating in these electrolytes. Furthermore, cage dynamics and potential of mean force calculations revealed the nature and strength of ion–solvent and ion–ion interactions, offering molecular-level insights into the transport and stability of glyme-based electrolytes for potassium-ion batteries. Figure 1 illustrates the chemical components used in the preparation of electrolytes.

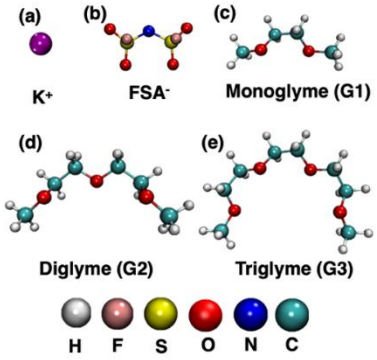


Figure 5 Chemical structure of molecules and ions used in this study.

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Theoretical studies of Indole oxidation by Biomimetic and Enzymatic systems using dioxygen.

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Dioxygenases are a fascinating class of enzymes that catalyze the incorporation of both atoms of molecular oxygen into organic substrates, initiating their metabolism.[1] Indoleamine 2,3-dioxygenase (IDO) and tryptophan 2,3-dioxygenase (TDO) are heme-containing dioxygenases that oxidize L-tryptophan (L-Trp) in the presence of O_2.[2] To elucidate their reaction mechanism, T.K. Paine and co-workers studied the reactivity of a biomimetic iron(II) complex, [$(TpPh_2)Fe^{(2+)}(OTf)(CH_3CN)$], which catalyzes the C–C bond cleavage of 2,3-dimethylindole (2,3-DMI). Unlike most previously reported biomimetic complexes that proceed via an Fe(IV)=O intermediate, no experimental evidence for such a species was observed in this system. Motivated by this unusual finding, we investigated the mechanism using density functional theory (DFT). Our results show that the reaction begins with substrate coordination to the metal centre, most favourably via dissociation of the acetonitrile and triflate ligand, consistent with ^{19}F NMR studies. Furthermore, we identified a minimum-energy pathway for 2,3-DMI oxidation to N-(2-acetylphenyl) acetamide via iron-superoxo and peroxo intermediates. Finally, the high turnover number is rationalized by a low-energy barrier pathway for regeneration of the Fe(III) species through single-electron transfer (SET) between two Fe(II) intermediates: the substrate-bound complex and the iron(II)-superoxo species.

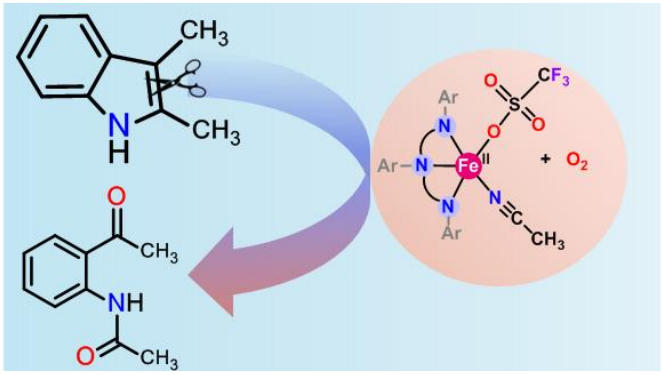


Figure 1 Schematic representation of proposed reaction mechanism for 2,3-DMI oxidation using iron complex.

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Theoretical Chemistry Symposium
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EFFECT OF GLYCOSYLATION ON THE CONFORMATIONAL DYNAMICS OF THE CATALYTIC DOMAIN OF HUMAN CARBONIC ANHYDRASE IX

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The enzyme human carbonic anhydrase IX (HCA IX) is a multi-domain, dimeric protein where glycosylation of its catalytic domain has been linked to its unique role in promoting the survival of malignant cells of solid tumors under low pH conditions. In the present work, we probe the role of glycosylation in terms of possible coupling of conformational fluctuations of the glycan chain to functionally important dynamics of the enzyme.[1] In the glycosylated monomeric and dimeric forms of the catalytic domain of HCA IX (HCA IX-c), the glycan chain is predominantly found in an extended conformation oriented towards the bulk solvent. Enhanced sampling leads to the identification of rare conformations back-folded towards the protein surface they transiently hydrogen bond to where several surface-exposed polar amino acid residues of the protein. Some of the back-folded structures hydrogen bond to $Glu-106$, indirectly connecting to the reactive proton transfer pathway essential for the enzyme's catalytic activity as shown in Figure 1.[2] In dimeric HCA-IX-c, the two glycan chains simultaneously form the rare backfolded and half-backfolded conformations. The observed correlation between glycan chain fluctuations and the reorganization dynamics at the active site is further investigated to reveal allosteric cross-talks[3] between the glycan chain and $His-64$, an amino acid residue critical for catalysis

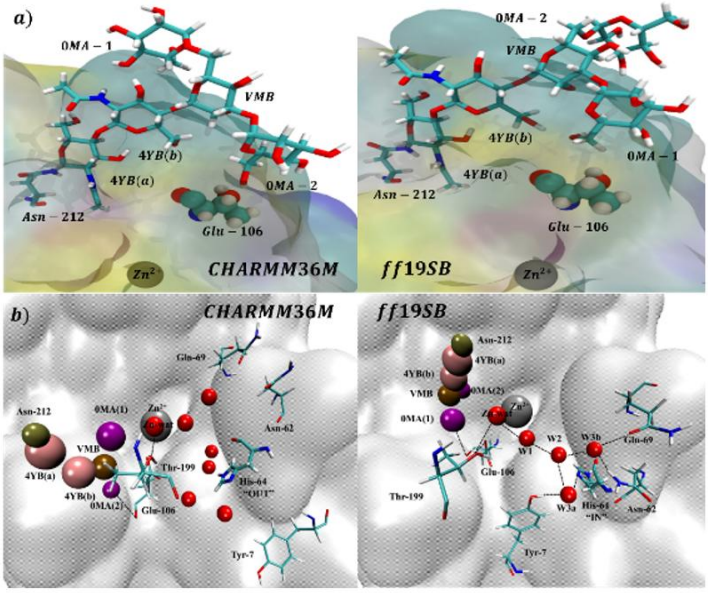


Figure 1: (a)Back-folded glycan chain conformations (b)Transient proton transfer network when the glycan chain is in back-folded conformation when two different force fields are employed.

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Unveiling the Structural, Magnetic, and Electronic Characteristics of an Extended Perovskite Material: A Theoretical Perspective

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Modern materials research is increasingly focused on emerging quantum and advanced materials, whose intricate physicochemical properties are key to enabling future breakthroughs in energy, electronics, and quantum technologies. Among these, perovskite oxides have emerged as a promising class of solid-state materials, largely due to their remarkable structural versatility, complex energy landscapes, and intriguing functional properties[1-3]. Although crystallographic constraints limit the structural variations of conventional 3D perovskites[4,5], doubling the perovskite unit cell significantly expands the available chemical space. This structural extension enables tunable electrical properties and exotic magnetic ordering, making these materials highly multifunctional and strong candidates for next-generation spintronic devices. In this symposium, we will present our recent advances in understanding structure-property correlations, including crystal-structure data-mining schemes, and the investigation of spin-ordering and electronic structure systematics through first-principles theoretical calculations that incorporate models accounting for strong electron correlations, relativistic effects, and hybrid functionals for a progressive class of double perovskites[6-8].

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Theoretical Chemistry Symposium
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Evaluating multi-state free energy profiles from splitting probability

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Single molecule experiments monitor the structural transitions of biomolecules under a constant mechanical force to study their fold–unfold transitions. The activation barrier for such transitions is obtained by inverting the observed committor, which is the probability that the molecule starting from a given extension reaches the folded state before the unfolded state. This work proposes an analytical model for committor analysis of the multi-state conformational dynamics of a DNA hairpin in a complex cellular environment, within the framework of the generalized Langevin equation using a general asymmetric bistable potential with a power-law frictional memory kernel. We obtained exact analytical expressions for the probability density function, first passage time distribution, and the committor. The results are compared with those obtained from steered molecular dynamics simulation of a three-state DNA hairpin, and earlier experimental data. We investigated the dependence of the committor and the corresponding committor-inverted profiles on the linker stiffness, barrier height, and degree of asymmetry in the bistable potential. This model successfully captures the fold–unfold dynamics, reproducing the multi-state free energy profile with asymmetric energy barriers.

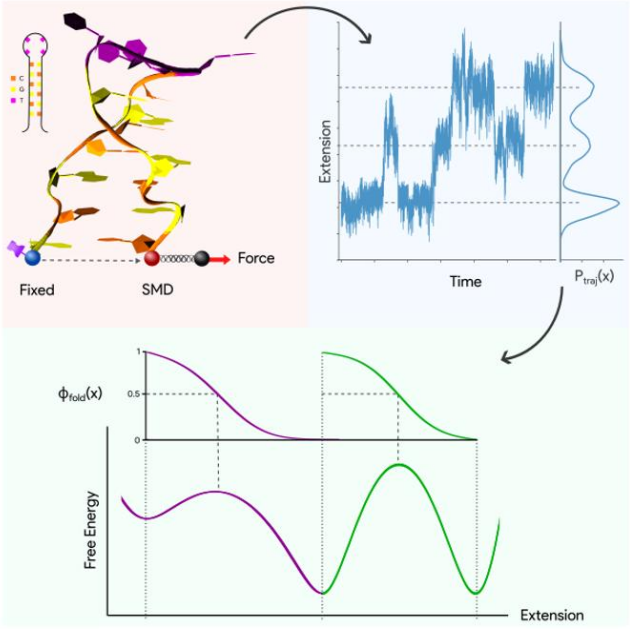


Figure 1: General Scheme

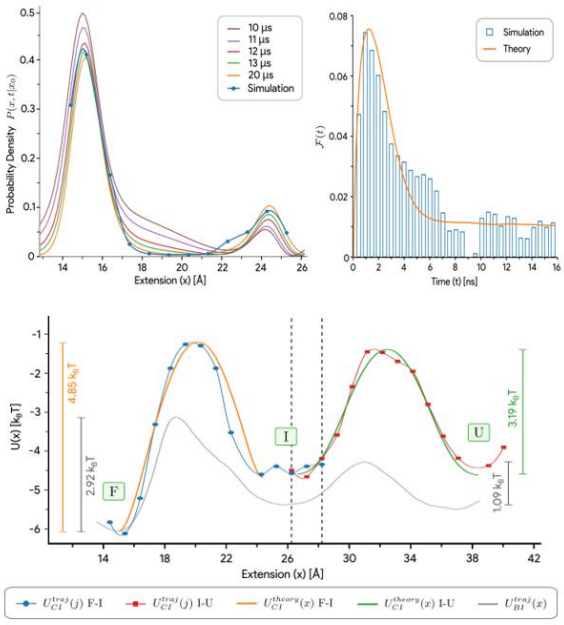


Figure 2: Results *(PDF, FPTD, and PMF)*

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Computational Investigation of Na-Decorated Functionalized Hydrogen substituted Graphdiyne toward Gas Capture and Sensing

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Air pollution arising from the rapid increase in automobile usage, particularly diesel-powered vehicles, remains a critical environmental concern. Exposure to diesel emissions has been shown to pose greater health risks, with toxic nitrogen oxides (N_2, N_2O, NO, and NO_2) directly implicated in cardiovascular diseases and chronic respiratory conditions such as chronic cough, asthma, bronchitis, and even cancer. Therefore, effective tracing and trapping of these molecules are essential for safeguarding public health. In this study, we have explored functionalized hydrogen-substituted graphdiyne (HsGDY) decorated with Na atom as a potential adsorbent material for gas sensing applications. Using density functional theory (DFT), the structural stability, adsorption behavior, and electronic properties of Na-decorated functionalized HsGDY were systematically investigated. Total density of states (TDOS) analysis reveals that gas adsorption induces a pronounced reduction in the energy gap, thereby enhancing electrical conductivity. Partial density of states (PDOS) results confirm orbital overlap between gas molecules and the functionalized slab, indicative of strong adsorption. Furthermore, non-covalent interaction (NCI-RDG) analysis highlights the role of weak interactions in gas capture, while charge density and Löwdin charge transfer studies emphasize significant electron redistribution upon adsorption. Recovery time calculations demonstrate rapid desorption with temperature variation, ensuring reusability of the material. Overall, these findings establish Na-decorated functionalized HsGDY as a highly efficient and selective two-dimensional carbon-based material for detecting and capturing nitrogen and its oxides, offering a promising pathway toward advanced gas sensing technologies and sustainable environmental remediation.

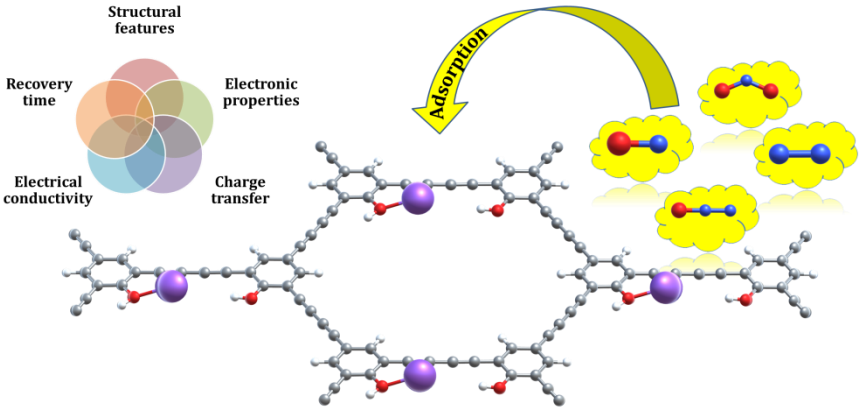


Figure 1. Schematic representation of tracing and trapping nitrogen and its oxides on Na decorated OH-HsGDY

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Barrier-Controlled Thresholds Underpin Non–Michaelis–Menten Kinetics

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Enzymes drive nearly all biological processes by accelerating reactions with remarkable efficiency. The classical Michaelis–Menten (MM) model[1] was highly successful in explaining early observations by showing that enzyme rate increases monotonically with substrate concentration, rising in a hyperbolic fashion toward saturation. Experimental studies have shown that many enzymes do not follow the smooth, hyperbolic behavior predicted by MM kinetics. Instead, they can switch between slow and fast activity regimes. In GroEL/GroES, low substrate load keeps the system in long resetting cycles (slow), while higher load promotes productive turnover (fast)[2,3]. In RNA polymerase (RNAP), activity shifts between a fast elongation regime and a slower paused or backtracked regime, with higher NTP concentrations favoring the fast mode and lower levels or regulatory inputs stabilizing the slow mode[4,5]. We approach this problem using a free-energy landscape framework that explains how enzymes redistribute flux between slow and fast routes as substrate levels and conformational barriers change. A compact deterministic treatment identifies the boundaries between slow and fast regimes, while stochastic simulations capture the fluctuations and waiting times that are hidden in bulk measurements. Together, these results show that enzyme activity can display two distinct plateaus with a sharp, substrate-dependent switch between them. The position of this switch is set by a gating barrier, linking microscopic features of the landscape to the observed kinetic behavior. Overall, the framework provides a clear explanation for non-classical MM kinetics and identifies experimental approaches—such as substrate-depletion protocols and mutational studies designed to shift conformational states, to test and refine the model.

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Theoretical Chemistry Symposium
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Unraveling the Regioselective Reaction Mechanism of Gentisic Acid Catalyzed by SDO Enzyme

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Salicylate 1,2-dioxygenase (SDO), a ring-fission non-heme dioxygenase enzyme, displays a unique regioselective reaction with gentisic acid (GTQ) in the presence of molecular oxygen. Classical molecular dynamics simulations were carried out for both the wild-type SDO and its mutated variants, Asp174Glu and Asp174Ala, revealing the presence of three active water molecules at the enzyme's active site, pivotal in facilitating the oxidative cleavage of an aromatic C–C bond in the GTQ substrate [1]. Additionally, employing quantum mechanics/molecular mechanics (QM/MM) calculations, we unveiled three distinct reaction mechanisms explaining the regioselective oxidation of GTQ by the SDO enzyme. The formation of the main product, maleylpyruvate, via pathway A emerged as the most favorable mechanism, with a rate-determining barrier of 21.4 kcal mol^{-1}. Our study underscores the essential role of active water molecules in stabilizing the O_2 molecule and aiding in O–O and C–C bond cleavage, while also highlighting the crucial anchoring function of Asp174 in the enzymatic cycle. Moreover, upon introducing the G106A mutation to the wild-type enzyme, a significant change in catalytic activity was observed with two different substrates, salicylate and GTQ, attributable to the presence of a hydrogen bond network with water and the 5'-OH group of GTQ, which is absent in salicylate [2]. Long-range classical molecular dynamics simulations of both the wild-type SDO and its G106A mutant variant, each complexed with two different substrates, confirmed the existence of an inter molecular hydrogen bond network which is aligned with previous findings.

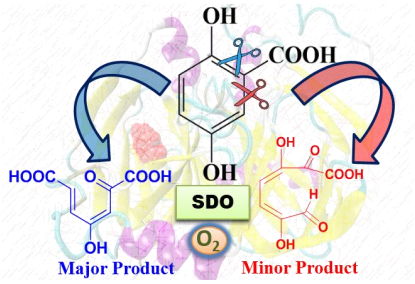


Figure 1 Dioxygenase activity of SDO on substrate GTQ.

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Mechanistic insights into hydroxyl radical initiated oxidation of aminocarb

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Abstract:

Aminocarb (4-dimethylamino-3-methyl-N-carbamate) i6u46iyygcmb ms a carbamate pesticide widely used in agriculture and forest areas to control insect populations. It disrupts the nervous system of insects, causing overstimulation, paralysis, and eventual death (1). Although aminocarb is used as an effective pesticide to control the insects, it also directly affect the non-target organisms, including birds, predatory insects, pollinators, and mammals in the environment (2). Understanding its degradation pathways is therefore crucial to assess its long-term impact on human health and the environment. In the present study, the reaction of OH radical with aminocarb is investigated using the density functional theory (DFT) methods, M06-2X and ωB97XD with 6-31+G(d,p) basis set. A total of eight H-atom abstraction, twelve OH radical addition and one dissociation reaction pathways are identified. At 298 K, the calculated overall rate constant for the initial reactions is found to be 1.83 x 10^{-10} $cm^3molecule^{-1}s^{-1}$, indicating that the reactions are significantly faster. The alkyl radicals formed in the favourable initial reactions readily react with O_2 to form a peroxy radical. Then, the peroxy radical undergoes a further oxidation process which leads to the formation of closed shell products. These findings will provide mechanistic insights on the degradation of aminocarb, and its impact on the environment.

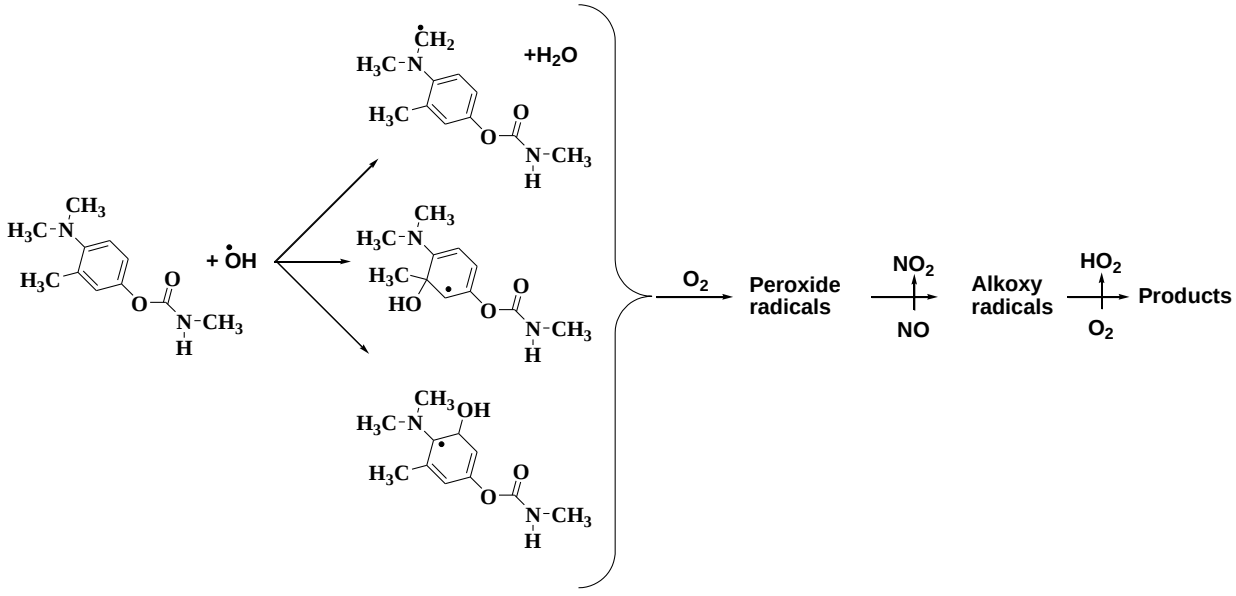


Figure 1 The reaction mechanism for the OH radical initiated oxidation of aminocarb

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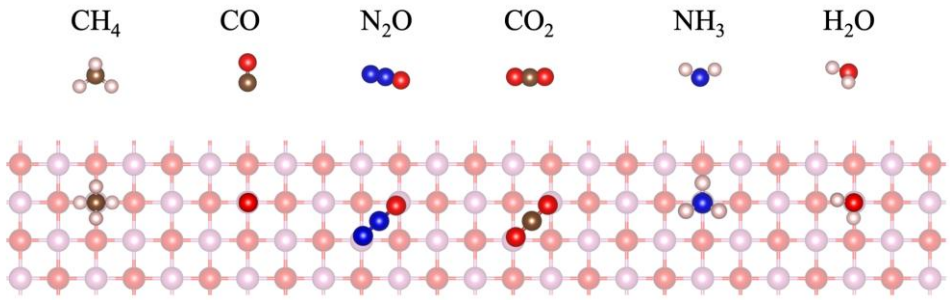
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Density Errors in Molecule-Surface Interactions and How to Correct Them?

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The primary workhorse of surface chemistry, dispersion-corrected Kohn-Sham (KS) density functional theory (DFT) methods, offer only semi-quantitative description of molecule-surface interactions, necessitating the use of computationally expensive correlated wavefunction based methods to obtain accurate results.[1,2] The random phase approximation (RPA) based methods developed in a computationally efficient post-(KS) formalism are known to perform well in describing most of the chemical systems, while for the case of molecule-surface interactions result in underestimation[3], speculated to be the result of density driven errors. Recently developed RPAS, a time-dependent Hartree-Fock (TDHF) Hessian based perturbative density correction scheme for RPA, is known to improve the description of weakly bound closed and open-shell systems.[4] Here, we show that the RPA+RPAS approach improves the description of interactions between molecules and the MgO(001) surface. Similar improvements are achieved at the KS-DFT level using the HF density to correct the density-driven errors.[5] For the r^{2}SCAN-D4 functional[6,7], correcting for density-driven errors improves the interaction energies.



	CH_4	CO	N_2O	CO_2	NH_3	H_2O
RPA	27	125	85	82	49	69
RPA+RPAS+AXK	14	31	57	39	29	31
r^{2}SCAN-D4	-46	-100	-33	-71	-28	-88
r^{2}SCAN-D4@HF	-8	2	11	-9	21	-15

Figure 1. Errors in the interaction energy compared to MP2+ΔCC method, for different single molecule interaction with MgO(001) surface. AXK is a functional error correction to the RPA energy. All values are in meV.

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High-throughput screening of single atom catalysts for oxygen reduction reaction

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For the oxygen reduction reaction (ORR), heme-based single-atom catalysts (SACs) have garnered a lot of attention. However, catalytic performance is limited by their weak electrochemical stability. Motivated by reports of non-heme-based SACs in electrocatalysis, we conduct a density functional theory (DFT) analysis of 112 heme and non-heme SACs comprising salen, corrole, and confused porphyrin frameworks with various transition metals (Sc, Ti, V, Cr, Mo, W, Mn, Fe, Ru, Os, Co, Rh, Ir, Ni, Cu, and Zn) adsorbed on the graphene surface. We evaluate the activity and stability of the SACs using a five-step high-throughput screening approach. After analysing the thermodynamic stability, about 63 SACs are obtained with optimum binding of the intermediates. Mean-field micro-kinetic modeling is carried out in the third phase, which provided around 19 SACs as having good activity as Pt(111) surface. The Pourbaix stability study and pH-dependence calculation led to the screening of 16 SACs with good activity and stability for ORR.

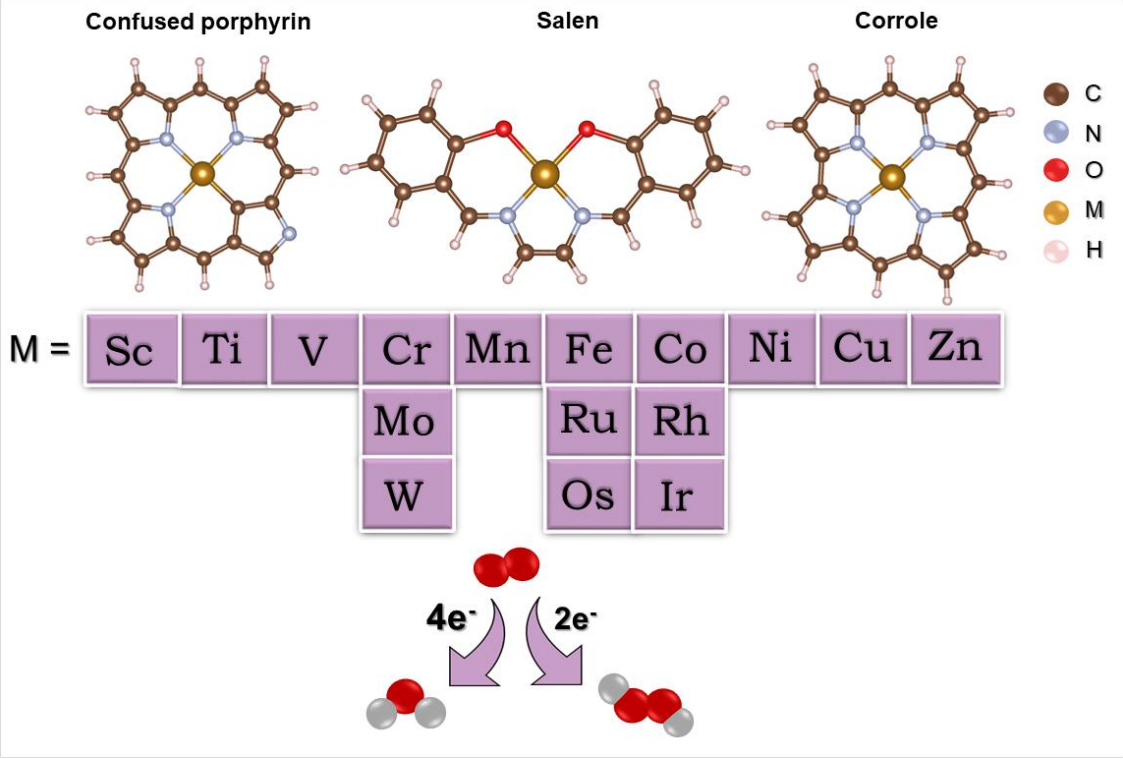


Figure 1 Structure models of the SACs embedded onto the graphene support with various transistion metal dopants for ORR

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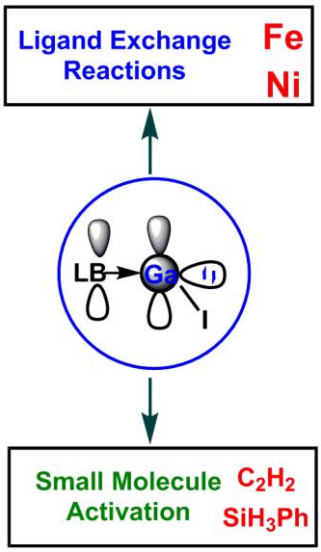
Mono(Lewis Base)-Stabilized Gallium Iodide: An Unexplored Class of Promising Ligands

Sahtaz Ahmed,[a] Himashri Das,[a] Daniel González-Pinardo,[b] Israel Fernández*[b] and Ashwini K. Phukan*[a]

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Quantum-chemical (DFT) calculations on hitherto unknown base(carbene)-stabilized gallium monoiodides (LB→GaI) suggest that these systems feature one lone pair of electrons and a formally vacant p-orbital – both centered at the central gallium atom – and exhibit metallomimetic behavior. The calculated reaction free energies as well as bond dissociation energies suggest that these LB→GaI systems are capable of forming stable donor-acceptor complexes with group 13 trichlorides. Examination of the ligand exchange reactions with iron and nickel complexes indicates their potential use as ancillary ligands in transition metal chemistry. In addition, it is found that the title compounds are also able to activate various enthalpically robust bonds. Further, a detailed mechanistic investigation of these small molecule activation processes reveals the non-innocent behavior of the carbene (base) moiety attached to the GaI fragment, thereby indicating the cooperative nature of these bond activation processes. The energy decomposition analysis (EDA)[1] and activation strain model (ASM)[2] of reactivity were also employed to quantitatively understand and rationalize the different activation processes.



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Spectral Tuning in Cyanobacteriochrome

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Phytochromes are photoreceptors that play a crucial role in regulating various physiological activities in plants and bacteria, such as phototaxis, gene expression and photosynthesis [1]. In addition to a central chromophore, phytochromes comprise of a large protein environment. This protein environment has a significant role in dictating the absorption properties and in overall photocycle in different species. In canonical phytochromes, the resting state (Pr) absorbs the red light (700 nm), while the end photoproduct (Pfr) absorbs at the far-red region of the spectra (754 nm). However, in cyanobacteriochromes (CBCRs) surprisingly it has been seen that the resting state, Pr though absorbs at the red region (649 nm) the final state of the chromophore (Pg) absorbs in the green region (536 nm) [2]. So, unlike the canonical counterpart, CBCR shows a large blue shift in the absorption pattern of the end species of the photocycle.

By employing hybrid QM/MM approaches, we attempt to understand the reason behind such differences in absorption patterns. We believe that differences in absorption patterns come about because of different structural effects on the chromophore exerted by the protein environment. Understanding the details of such interaction will help these photoreceptors to emerge as a promising source of optogenetic tools [3] in near future.

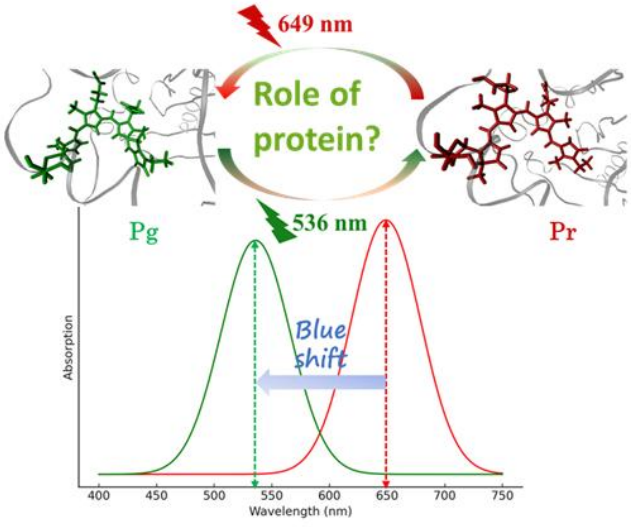


Figure 1 Schematic representation of spectral shift in CBCR.

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Atmospheric Reaction of Hydroxymethyl Methyl α-Lactone (HMML) with OH Radicals and Cl Atoms

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Isoprene, a major biogenically emitted volatile organic compound (VOC), oxidizes in the presence of NO to yield hydroxymethyl methyl α-lactone (HMML). Although the aqueous-phase chemistry of HMML has been studied, its gas-phase chemistry has remained unexplored.[1] This study computationally investigates the thermodynamics and kinetics of HMML oxidation by OH radicals and Cl atoms in the gas phase. The oxidation proceeds via exothermic hydrogen atom abstraction. Potential energy profiles for all reaction pathways were constructed at CCSD(T)//M06-2X/6-311++G(d,p) level of theory.[2] The rate constants were calculated using variational transition state theory with tunneling corrections over 200–400 K.[3] At 298 K, HMML's atmospheric lifetime is 9.6 days in the marine boundary layer and 62.5 days in the troposphere. Degradation studies of product radicals resulted in end products with shorter lifetimes, including α,β-unsaturated carboxylic acids, formic acid, pyruvic acid, methylglyoxal, and diketones.[4]

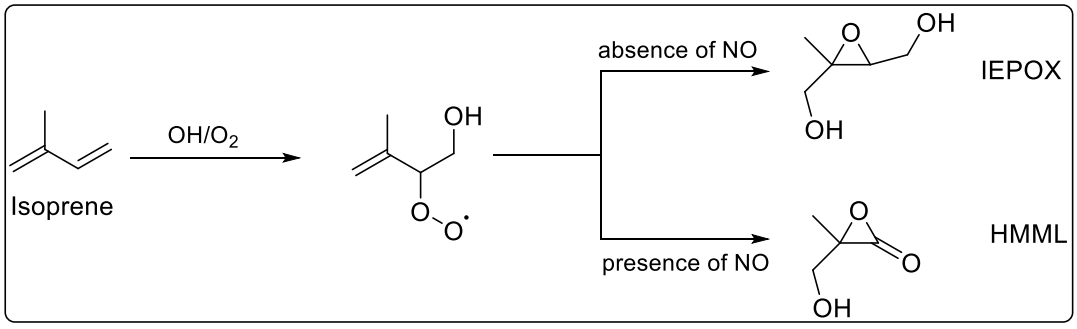


Figure 1: Oxidation of isoprene initiated by OH radicals in the presence of O_2 and NO yields HMML, while in the absence of NO it yields IEPOX.

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State-dependence in diffusion-controlled transport and stochastic resonance

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Most natural phenomena evolve through non-equilibrium pathways following non-linear dynamics involving the crossing of a potential energy barrier. During these processes the systems transit from one state to another. We intend to understand in detail the significance of these states, their positions, and associated intrinsic fluctuations. As these systems are inevitably subjected to environmental noise, there appears complexity in studying their behavior. We focus on analyzing the rate of diffusion-controlled transport in these complex systems under pertinent conditions. We implemented distinctions in the characteristics of the concerned states by altering their positions and the level of noise or diffusion coefficientslinked to them. It has been observed that the variation of the reference point position and the diffusion coefficients have significant impacts on the rate. Our investigations unveil very important and critical aspects of the characteristic roles of the initial and final states in diffusion-controlled kinetics. We continued to develop an understanding of these fundamental transport phenomena where periodic force is involved. This is a particular scenario where the constructive interplay of noise and the non-linearity of the system comes into effect in the presence of appropriate conditions. The phenomenon is termed stochastic resonance. We explored the significance of the state dependence in stochastic resonance which manifests in many natural and designed processes, starting from climate systems to chemical reactions1-3 . We developed a completely analytical theory in the adiabatic limit and a semi-analytical approach for the general case for stochastic resonance considering state-dependent diffusion. The theoretical findings are substantiated with numerical simulation results. The results of our studies not only enrich the fundamental understanding of diffusion-controlled kinetics but also indicate the paths to developing advantageous technologies based on optimizing the conditions of transport.

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In Sillico Study of the Fusion of Photochemical Olefin Metathesis and Amination Reaction

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Olefin metathesis is a versatile and efficient method for C–C double bond formation, broadly applicable in synthetic, medicinal, and materials chemistry for constructing complex molecular architectures.[1] Herein, a fusion of photochemical olefin metathesis with a C-H amination reaction has been crucially studied for the generation of amine functionalized olefin. Our study unfurls the handling multiple demands of a photocatalysis such as N-O bond cleavage of an oxime ester **a** to produce N-centered radical (NCR) **c** through energy transfer (EnT) and benzoyl radical followed by single electron oxidation (SET) generates benzoyl anion. Along with this on the other side a simultaneous cyclobutane analogue **d** is formed due to a pi-pi stacking interactive orientation between two styrene moieties through [2+2] cycloaddition. Through a ring-opening olefin metathesis process Z-stilbene radical cation **f** forms which is stabilized by previously generated benzoyl anion (cation-anion interaction) followed by a stereo-selective amination reaction. *In Situ* generated benzoic acid catalyzes here in N-H protonation of the 1,3-H shifted imine followed by another SET with a simultaneous benzoyl radical elimination results in the final outcome **Pdt** (Figure 1).[2,3]

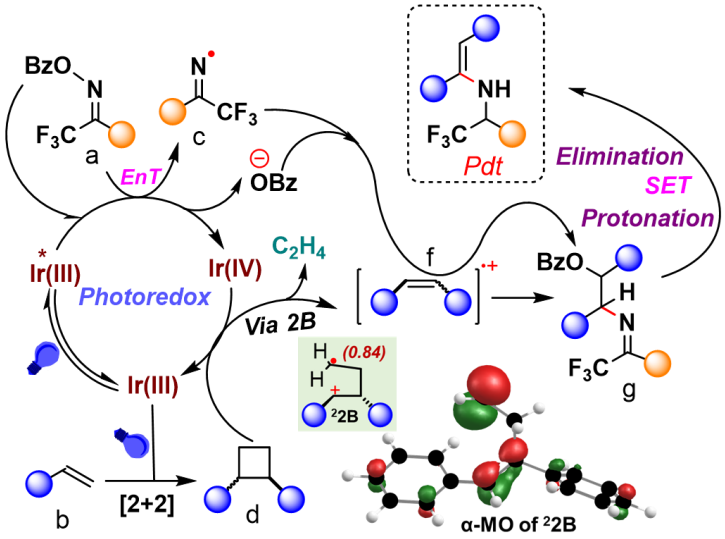


Figure 1: Proposed Reaction Mechanism for the Formation of Z-selective aminated stilbene (**Pdt**) from Oxime ester **a** and Styrene **b**. Inset: Spin density plot with population value of **2B**

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Chemical Space Exploration of Synthesizable organic D-A TADF Emitters

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Thermally activated delayed fluorescence (TADF) materials have gained attention as promising emitters for organic light-emitting diodes (OLEDs), enabling up to 100% internal quantum efficiency without the need for costly noble metals. Nevertheless, the development of high-performance TADF emitters remains challenging, largely due to the intricate relationship between molecular architecture and key photophysical parameters—especially the singlet–triplet energy gap, delta E_{ST} and the oscillator strength (f).[1] In this work, we present a comprehensive computational workflow for exploring the chemical space of donor-acceptor TADF molecules. We constructed a focused library of experimentally validated donor and acceptor scaffolds, ensuring practical synthetic accessibility. The combinatorial assembly of these building blocks generated a diverse yet realistic molecular space. Ground state geometries were optimized using a machine learning potential (MLIP) trained on wB97M-D3BJ def2-tzvpp quantum mechanical calculations. Excited state properties were computed using time-dependent density functional theory (TD-DFT) single-point calculations at the optimized S_0 geometries.

This approach successfully identified several promising candidate molecules that possess both a small singlet-triplet energy gap (ΔEST) and sufficient oscillator strength for efficient emission. To assess their practical viability, an autonomous agent evaluated these candidates by calculating their **synthesizability scores** and performing computational **retrosynthesis** to map potential synthetic routes.Our workflow demonstrates the power of combining physical insights with machine learning for the rational design of TADF emitters. This methodology can be readily extended to other molecular property optimization challenges in organic electronics.



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A First-Principles Study of Silicene on Ag(111) Surface

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Silicene, a graphene-analogous two-dimensional material composed of silicon atoms, can be synthesized via Molecular Beam Epitaxy (MBE) on Ag(111) substrates, leading to low-buckled sheets [1]. Extending this method to grow multilayer films has demonstrated improved air stability compared to monolayers [2] —an essential advancement toward silicene-based field-effect transistors [3].

In this work, we employed high-performance computing resources to perform *ab initio* Density Functional Theory (DFT) calculations using the Quantum ESPRESSO package. Various configurations of silicon atoms — ranging from isolated adatoms to sub-monolayer and multilayer arrangements—were modelled over a slab geometry of Ag(111). The slab approach enabled accurate simulation of surface behaviour through selective atomic relaxation across layers. To understand the strain-induced reconstructions of silicene on Ag(111), we modelled the system's sub-monolayer cluster region. We performed systematic geometrical relaxations for silicon clusters of various sizes within the Ag(111) supercells constructed to match the experimentally observed *(4x4)*[1] and *$(2\sqrt{3}x2\sqrt{3})R30^0$* [4] structures. This method yielded stable structural parameters and provided detailed structural insights of the surface structure in various cluster sizes. Furthermore, by calculating the interaction energy per Si atom as a function of cluster size, we mapped the energetics that governs the reconstructed Silicene surfaces.

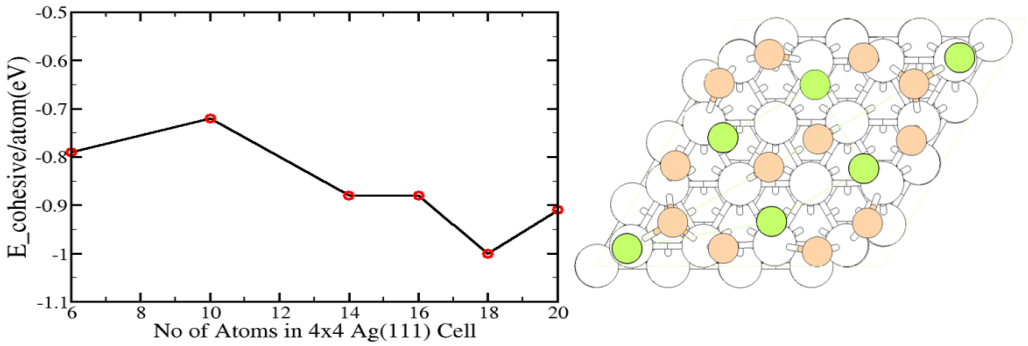


Figure 1 Cohesive Energy-No of Atoms in Cluster Plot and Top View of 18 atom 4x4 Reconstructed Silicene

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Theoretical Chemistry Symposium
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Effect of Metal based Anion in Ionic Liquid@UiO-66 MOF for Selective CO_2 Capture and Separation: A Computational study

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The carbon capture from flue gases is an important step to fight global warming and climate issues due to the fact that CO_2 is consider to be a main cause for global warming [1]. In past decade researches were carried out to identify a potential candidate for CO_2 capture and separation from the flue gas. Ionic Liquids (ILs) and metal organic framework (MOF) are two well-known materials in the field of CO_2 capture [2,3]. In this work we have selected UiO-66, a Zirconium based MOF with several ILs which has common cation as $[EMIM]^+$ and various anions such as $[Cl]^-$, $[AlCl_4]^-$ and $[FeCl_4]^-$. To understand the effect of metal-based anion in CO_2 capture and its selectivity over other gases, selected ILs were impregnated in *Octahedral* (*Oh*) and *Tetrahedral* (*Td*) pores of UiO-66 [4]. It is found from calculations that the selectivity of CO_2 increases with increase in spatial confinement. Heat of adsorption of CO_2 is relatively higher for $[EMIM]^+$ $[AlCl_4]^-$ @ UiO-66 composite. Selectivity of CO_2/CH_4 and CO_2/N_2 was evaluated for selected ILs@UiO-66 composites. Our study will depict a molecular level understanding towards effective CO_2 capture and its separation.

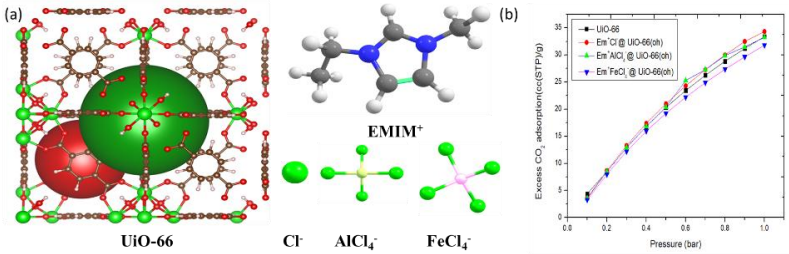


Figure 1 (a) UiO-66 with two different pores and Selected ILs, (b) Single adsorption isotherm of CO_2 on selected materials.

References:

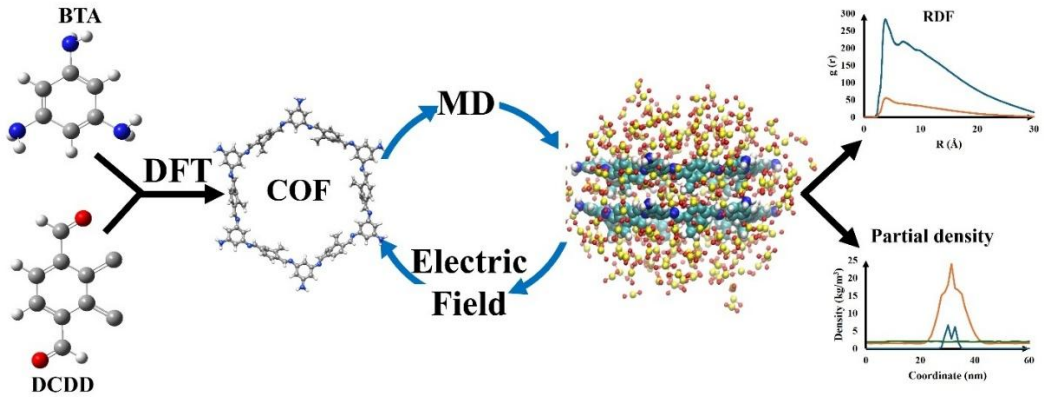
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DFT and MD Simulations Study of Covalent Organic Frameworks for Selective SO_2 Capture and Sustainable Gas Separation

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Rapid industrialization and technological advances have led to high levels of discharge of hazardous gases. Sulfur dioxide (SO_2) is one of the gases that severely affects the environment, leading to acid rain and corrosion of industrial infrastructure. Thus, designing advanced materials capable of selectively capturing and recovering SO_2 from mixed gas streams is of critical environmental importance. Covalent organic frameworks (COFs), known for their high surface area, tunable pore sizes, functionalized pore walls, and excellent thermal and chemical stability, have emerged as promising candidates for gas separation. Although COFs have been widely studied for CO_2 capture, their potential for SO_2 adsorption remains unexplored. In this work, a COF, designed from 5,6-dimethylenecyclohexa-1,3-diene-1,4-dicarbaldehyde (DCDD) and benzene-1,3,5-triamine (BTA), is investigated using a combined density functional theoretical (DFT) approach and classical molecular dynamics (MD) simulations. The DFT calculations at the B3LYP-D3/6-311+G(d) level revealed strong physisorption of SO_2 at electron-rich diene sites compared to that of CO_2. Bulk-phase MD simulations of SO_2-N_2, CO_2-N_2, SO_2-CO_2 supported the above findings. The radial distribution functions and density profiles indicated multilayer adsorption of SO_2, in contrast to CO_2, the latter showed monolayer adsorption.The studies on competitive adsorption of various gases demonstrated that, under mixed-gas conditions, both SO_2 and CO_2 are adsorbed with prominent adsorption of SO_2. On applying an external electric field, the adsorption of SO_2 is decreased. The present study highlights the potential of the designed DCDD-BTA-based COF for efficient and selective SO_2 capture, using electric fields as a regeneration stimulus, offering new opportunities for gas separation and environmental remediation technologies.



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Cooperative and Anti-cooperative Effects in Osme Bonded OsO_4-Pyridine Complexes Induced by H_2O Molecule

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This theoretical investigation focuses on the relatively underexplored metal-centered non-covalent interaction known as the "Osme bond"[1,2], formed between X-Pyridine (X = -NH_2, -CH_3, -F, -CN, -NO_2) and OsO_4. It examines how various substitutions on pyridine at para position affect the nature, strength, and cooperative characteristics of these interactions when H_2O molecule is made to interact with the binary complexes. Geometry optimization of the binary and ternary complexes was done using the ωb97x-D3 and LC-BLYP functionals in conjugation with def2-TZVP basis set. This work is divided into two sections. The first section focuses on the strength and electronic redistribution of Os…N Osme bonds in binary complexes, supported by AIM[3] and NBO[4] analyses. It is observed that the binding energies ranging from -39.05 to -26.47 kJ/mol, correlate strongly with descriptors such as proton affinity, ionization potential, and electron density at the bond critical point (BCP). The second section assesses cooperative versus anticooperative effects arising from the X-Pyridine.OsO_4 interaction with H_2O molecule. We identified two different sets of assemblies for the X-Pyridine•OsO_4•H_2O complexes. The most stable assembly features a cyclic interaction where H_2O interacts with both X-Pyridine and OsO_4 (as shown in Set I of **Figure 1**), leading to increased cooperativity. In contrast, the second assembly (Set II) shows a shift in interaction from a hydrogen bond to an Osme bond as substituents transition from electron-donating (ED) to electron-withdrawing (EW). These findings can be useful in enhancing our understanding of the critical features of the Osme bond and in facilitating the precise control needed to design materials with tailored properties for specific applications.

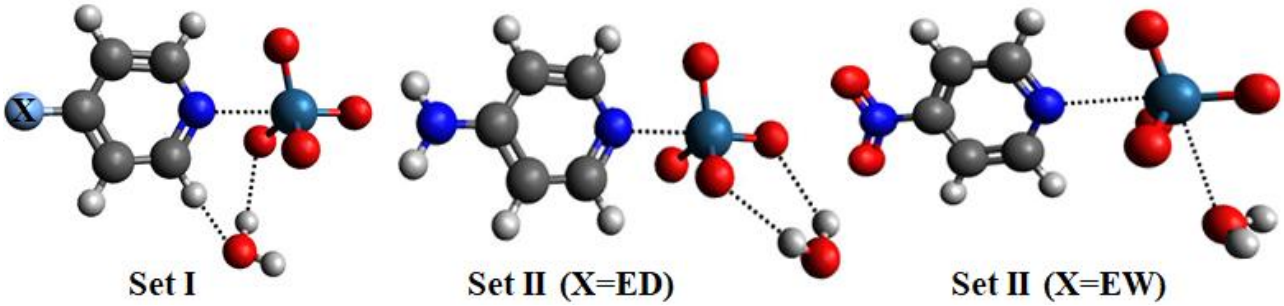


Figure 1 Pictorial representation of some X-Pyridine•OsO_4•H_2O ternary complexes.

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Redefining Dirhodium Catalysis: Experimental and Computational Evidence for Monorhodium as the Hidden Active Catalyst in Carbonyl Arylation

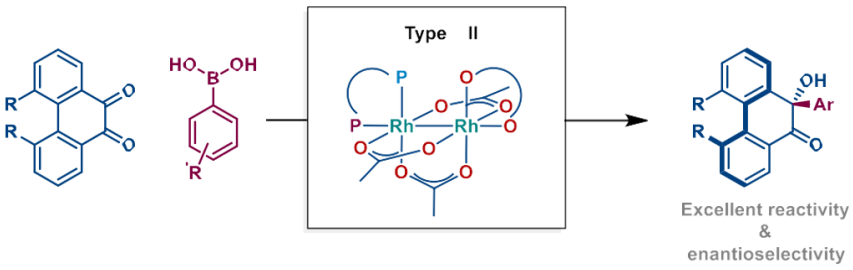
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Dirhodium paddlewheel complexes are versatile catalysts in diverse transformations. Their reactivity and selectivity can be easily tuned by modifying the bridging carboxylate ligand and anchoring ligands at axial sites. However, both approaches demand labor-intensive efforts. In 2010, Ma et al. first demonstrated that using an external NHC ligand could induce new reactivity by coordinating at the free axial site, albeit stereoselectivity remained poor.[1] In the few recent studies, dirhodium/bisphosphine revealed promising reactivity, with stereocontrol often substrate-specific.[3,4,5] Building on this ligand-directed strategy, Gu and coworkers (2023) reported high reactivity and enantioselectivity in carbonyl arylation, proposing a Type II complex as the active species, but direct evidence remained elusive.[2]

In this study, we combined synthesis, X-ray crystallography, VT-NMR, ESI-HRMS, and DFT to probe the mechanistic origin of carbonyl arylation. Our results show that the proposed Type II complex is catalytically inactive. Instead, we identify a transformation of the dirhodium precatalyst into a new monorhodium active species, directly observed for the first time. These findings reveal key structural and electronic factors governing reactivity and stereocontrol, providing a blueprint for designing next-generation enantioselective Rh catalysts.



Scheme 1. Carbonyl Arylation reaction catalyzed by Dirhodium/Josiphos catalysts.

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"Multi-Alkali Ion Storage and Diffusion Mechanisms in a Carbon-Based Anode: A First-Principles Study"

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CP-graphyne, a novel 2D carbon allotrope, exhibits excellent potential as an anode material for next-generation Li-, Na-, and K-ion batteries owing to its unique topology, high conductivity, and strong ion affinity.[1] First-principles calculations revealed favorable adsorption, stable voltage behavior, and efficient ion diffusion across the surface. AIMD simulations further confirmed its thermal and structural stability under operating conditions. Overall, CP-graphyne demonstrates remarkable adsorption, diffusion, and stability characteristics, highlighting its promise as a high-performance anode for multi-ion rechargeable batteries.

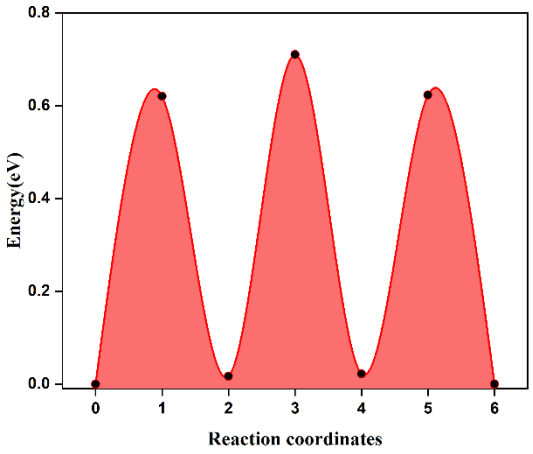


Figure 1 illustrates the nudged elastic band (NEB) image of the Li-ion migration pathway on the anode surface.

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Influence of Electron-Donating and Electron-Withdrawing Groups on Tuning the Energy Gap Between Ferrotoroidal and Antiferrotoroidal States in a Series of {$CrDy_6$} Complexes

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Toroidal states have emerged as promising candidates for next-generation technologies such as spin qubits, magnetoelectric coupling, spintronics, and quantum sensing. Despite their potential, stabilizing these states at the molecular level remains a significant challenge. Enhancing toroidal moments requires long-range vortex alignment or strong dipolar interactions to control magnetic anisotropy effectively. In our recent work on {MLn_6} complexes, we reported the first molecular system exhibiting a ferrotoroidal (FT) ground state. For practical applications, competing magnetic states must lie much higher, ensuring a large FT–AFT (antiferrotoroidal) energy gap. However, no established chemical strategies are currently available to increase this gap systematically.

To fine-tune this gap further, we introduced electron-donating (CH_3) and electron-withdrawing (Cl, Br, I) substituents at the para position of the o-toluic acid ligand in structurally related complexes. These modifications allow us to probe the impact of electronic effects on the FT–AFT gap. Single-crystal X-ray diffraction analysis of the modified complexes reveals changes in the height-to-radius (h/r) ratio, a key geometric parameter influencing dipolar interactions. A lower h/r ratio corresponds to stronger inter-triangle dipolar coupling, which in turn affects the FT-AFT gap.

Additionally, detailed DC and AC magnetic measurements, supported by *ab initio* calculations (CASSCF/RASSI_SO/SINGLE_ANISO/POLY_ANISO), confirm the presence of an FT ground state across the series. These findings demonstrate that electronic substituents and structural modulation can effectively fine-tune the FT–AFT gap, offering a viable chemical strategy for controlling toroidal magnetic behaviour at the molecular level.

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INVESTIGATIONS INTO RADICAL MOLECULAR SOLAR THERMAL SYSTEMS

Molecular Solar Thermal (MOST) systems offer an innovative and sustainable approach to energy storage and conversion, addressing key challenges in the global energy crisis. These systems are entirely metal-free, relying solely on purely organic compounds, which removes the need for rare earth elements or transition metals commonly used in conventional solar and battery technologies.

In MOST systems, both light absorption and energy storage occur within the same molecule via reversible photoisomerization, enabling efficient and compact energy conversion.
Their molecular tunability allows for precise control over absorption wavelengths, storage lifetimes, and thermal output.
Radical MOST systems in particular are promising due to an increased back-reaction barrier, stabilizing the the high-energy state and thus increasing the lifetime. We present an investigation into these systems and the challenges one faces when doing so.

Boosting the CO_2 reduction activity of Cu double atom catalyst through coordination environment engineering

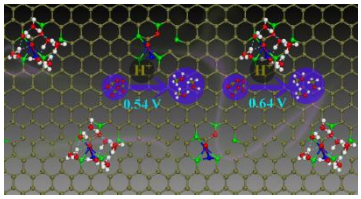
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Abstract: Double-atom catalysts (DACs) offer a reasonable and scalable route towards carbon neutrality owing to their efficient catalytic features. However, the challenges associated with the flexibility of their coordination structure usually restrict their full potential as efficient catalysts. Herein, we comprehensively examined the impact of coordination environment regulation on the CO_2R activity of Cu_2-DACs supported on C, N, or B co-doped graphene using ab initio simulations. We highlighted the marked role of the local coordination sphere of Cu_2-DACs in modulating their structural stability and charge transfer characteristics, thereby regulating the adsorption of CO_2 and various reaction characteristics. Notably, boron- and carbon-coordinated Cu_2 centres (Cu_2-B_xC_y) resulted in remarkably strong CO_2 adsorption (-0.65 to -2.31 eV), attributed to their amplified electronic interactions with the CO_2 molecule. The weak CO_2 binding observed on the carbon-nitrogen- and nitrogen-boron- coordinated Cu_2- centres (Cu_2-N_xC_y and Cu_2-N_xB_y) further highlighted the role of the coordination environment in facilitating the versatile binding modes of the key reaction species. The varying CO_2 interactions in these systems were further comprehended and supported by a multilevel descriptor (€) combining both geometric and electronic parameters. This descriptor closely mirrored the DFT results, thereby accentuating its effectiveness as a predictive tool to perfectly model the CO_2 interactions on these catalysts. Moreover, the dynamic behaviour in the adsorption modes led to partial breakdown of the conventional linear scaling relations between the key CO_2 reduction intermediates (*COOH, *CO, and *HCO). Among the numerous types of investigated electrocatalysts, Cu_2-B_5C_1 emerged as a highly active and selective catalyst for methanol production, with a remarkably low limiting potential of -0.54 V, surpassing the performance of several reported Cu-based systems. Besides, our findings underscored the often-overlooked yet crucial role of explicit solvation, which significantly altered both the potential-determining step and product selectivity. These outcomes emphasized the necessity of including solvation effects in realistic electrochemical modelling. Collectively, this study provides a critical mechanistic insight into better understanding the coordination effect on the CO_2R and a robust design strategy for next-generation Cu-based DACs, guiding the development of highly efficient and selective catalysts for CO_2 electroreduction

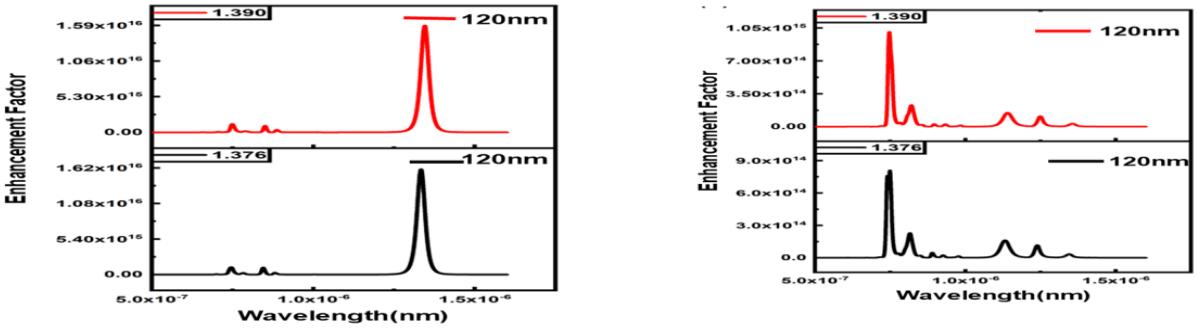


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Criss-Cross shaped Silver Nanostructure as Efficient SERS Substrates

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The performance of surface-enhanced Raman spectroscopy (SERS) in biomedical analysis is strongly governed by the plasmonic properties of the Raman scattering substrates. Therefore, the design and fabrication of high-performance SERS-active nanostructures remain crucial for advancing SERS technology[1,2]. In this work, we theoretically propose a crossed array of silver nanocrisscross structures on SiO_2 for direct detection assays, relying on favorable analyte–substrate interactions to yield strong SERS spectra upon analyte binding. Using the finite element method, both near-field and far-field enhancements of the crossed structures were analyzed. The near-field study reveals that intense electric fields are induced at the tips of the crisscross structures, leading to SERS enhancement factors on the order of 10^{16}, which can be tailored for specific SERS applications. Further optimization was achieved by tuning key geometrical parameters, including the width, thickness, and height of the crisscross arms in the monomer, as well as the gap size and asymmetry in the dimer arrays. Crisscross asymmetry in crossed dimers was introduced by varying structural dimensions along the x-direction, y-direction, or both, to improve the detection limit. Arraysof both symmetric and asymmetric crossed nanodimers were efficiently tuned to deliver strong SERS enhancements. The results highlight that silver based crisscross nanostructures exhibit higher SERS activity at shorter wavelengths, supporting their potential as reliable,miniaturized SERS sensor platforms for practical biomedical applications.

Figure 1. (a) and (c) The enhancement factors of asymmetric crisscross nanostructures (i and ii) under two different ri values: n=1.376 and n= 1.390.

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Theoretical Chemistry Symposium
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Computational and Matrix Isolation Infrared Spectroscopic Studies on Dehydroisoxazole Radicals

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The reactive and transient open-shell radical species that contain C, N, S, and O are of great interest in astrochemistry and astrobiology.[1] Additionally, free radicals are a significant class of classical reactive intermediates that extend their functions as polymer, biomolecular and molecular building blocks and in atmospheric and combustion chemistry.[2] Also, during metabolism, drug molecules with a lot of heteroatoms may produce radical species. We tried to study five-membered oxygen and nitrogen-containing isoxazole radicals using computational studies[3] in light of the significance of heterocyclic radicals. This included calculating the radical's relative energies, bond dissociation energies, spin density, NICSs, ELF, NBO, and RSEs. Furthermore, we studied 4-iodoisoxazole as the precursor that produces the corresponding isoxazole radical and looked into the photochemistry on 4-iodoisoxazole using matrix isolation infrared spectroscopy investigations in cryogenic settings. This contribution includes Density Functional Theory (DFT) calculations and preliminary findings of the photochemistry of 4-iodoisoxazole under matrix isolation conditions.

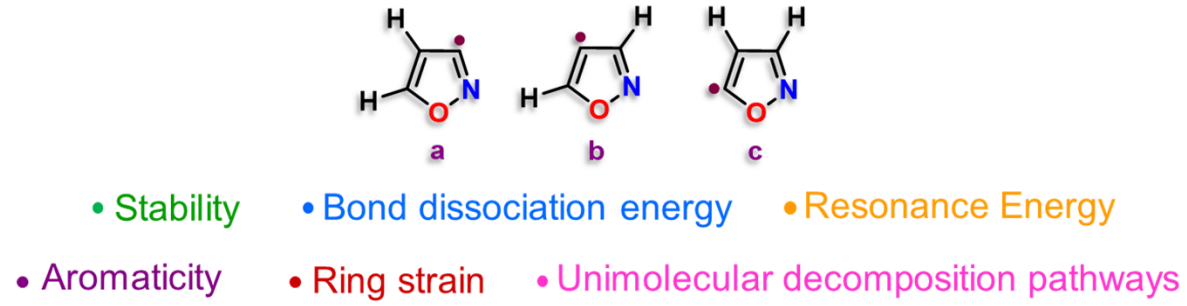


Figure 1. Isomeric radicals of Isoxazole (**a-c**)

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Understanding dissolution mechanism of oxide perovskites and activity tuning for O_2 evolution by surface doping

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Oxygen evolution reaction represents the major bottleneck in electrochemical water splitting. Development of efficient electrocatalysts from earth-abundant materials is essential.[1,2] This study reports a design principle for tuning the catalytic efficiency and stability of perovskite oxides, focusing on $SrMnO_3$, $SrFeO_3$, $SrCoO_3$, and $SrNiO_3$ through B-site surface doping with Mn, Fe, Co, and Ni metal ions. Owing to multiple active sites and tunable oxidation states, these oxide surfaces exhibit a considerable reduction in thermodynamic overpotential (η_{TD})[3,4] upon doping. Such trends are consistent with recent advances in thermodynamic and kinetic modeling of electrocatalytic reactions using first-principles approaches.[5] The dissolution free energy calculations are performed across a wide pH window (acidic to alkaline) and oxidative potentials to determine the Pourbaix stability and surface dissolution pathways. We find that $SrCoO_3$ and $SrNiO_3$ show the highest stability on doping with different transition metal atoms.

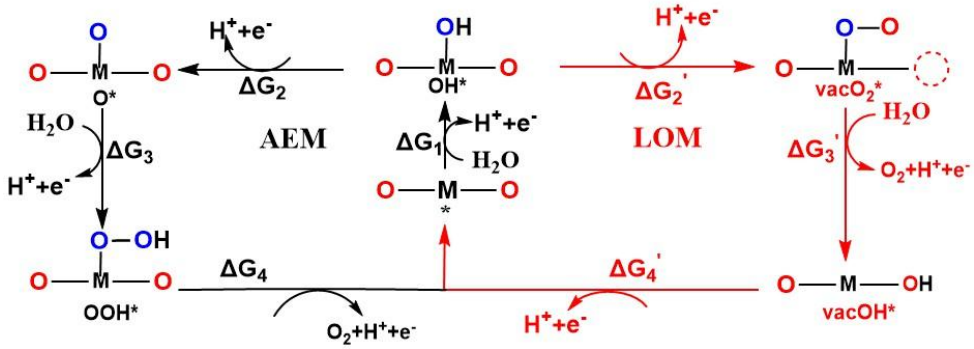


Figure 1. The adsorbate evolution mechanism (AEM) and the lattice oxygen mechanism (LOM) are illustrated. The black line represents the AEM pathway, while the red line corresponds to the LOM pathway. Each step proceeds through proton-coupled electron transfer, with the free energy changes denoted as ΔGi values.

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Electric Fields and Virtual Reality for Protein Design and Catalysis

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Electric fields play a fundamental role in enzymatic catalysis, guiding proton and electron transfer and stabilizing transition states and reaction intermediates.[1] Recent computational and experimental studies have demonstrated that local electric fields (LEFs) within enzyme active sites are not random, but evolutionarily optimized to enhance catalytic efficiency.[2] Understanding and visualizing these fields is therefore key to rational enzyme design and the creation of novel biocatalysts.[3] In our work, we have characterized and visualized electric field lines and proton transfer channels in natural heme peroxidases, such as ascorbate peroxidase (APX). Using molecular dynamics (MD) and hybrid QM/MM simulations, we mapped electrostatic networks that align with proton delivery pathways and redox-active centers. These maps were then brought into an immersive virtual reality (VR) environment, enabling us to intuitively explore the spatial organization of electric fields, trace proton transfer routes, and directly observe how electrostatic funnels guide catalysis across redox states. Building on these insights, we are now applying similar electrostatic and visualization strategies to *de novo* designed redox proteins.[4] In rationally engineered helical bundles such as *m4D2* and *e4D2*, we use VR-guided analysis to examine how targeted mutations reshape local field environments and influence redox behaviour.

By combining computational electrostatics with immersive molecular visualization, our work establishes a general framework for electrostatically guided, VR-enabled enzyme and protein engineering. This integration of physics-based design and interactive exploration links natural catalytic principles to emerging synthetic platforms, opening new possibilities for tailoring protein function through precise electrostatic control.

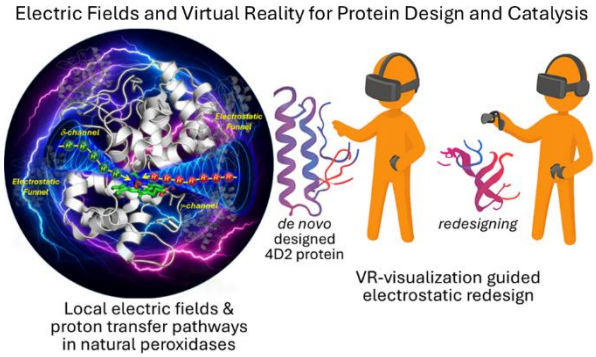


Figure 1. Visualizing and harnessing local electric fields for enzyme design: From mapping proton transfer channels in natural peroxidases to VR-guided electrostatic redesign of synthetic redox proteins.

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Theoretical Chemistry Symposium
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Ab-initio Study on the Hydrogen Bond of Water Dimer, Methanol Dimer and Water-Methanol Complex Under the Influence of External Electric Field (EEFs)

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Abstract

It is well established that external electric fields (EEFs) significantly influence the hydrogen-bond (H-bond) network in liquid methanol and methanol clusters, and can even induce proton transfer reactions [1]. However, describing molecules and clusters under EEFs remains challenging due to the non-local nature of density functional theory (DFT) functionals [2]. Therefore, benchmarking small molecular systems under EEFs is necessary.In this work, we present a detailed *ab initio* investigation of the structural changes and energetics of the methanol dimer and its fluorine-substituted analogues under EEFs of varying strengths, using both DFT and coupled-cluster with singles and doubles (CCSD) theory. To further assess the role of electronic forces, we analyze intermolecular interactions in three different dimers—water, water–methanol, and methanol—under applied EEFs. Overall, this study provides new insights into the nature of H-bonding interactions in methanol and related systems under the influence of external electric fields [3].

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Theoretical modelling of strongly correlated excited states of INVEST OLED molecules

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The unexpected violation of Hund's rule in certain N-heterocyclic chromophores, such as cyclazine and its derivatives, is often linked to an intriguing inversion of their low-lying excited singlet (S_1) and triplet (T_1) states [1,2]. This anomalous behavior, characterized by a negative singlet-triplet energy gap ($\Delta E_{ST} = E(S_1) - E(T_1)$), positions these molecules as promising candidates for next-generation OLED materials. Specifically, they serve as templates for fifth-generation OLEDs, leveraging reverse intersystem crossing (RISC) to enhance quantum yield via thermally activated delayed fluorescence (TADF). These so-called INVEST systems exhibit a delicate interplay of static and dynamic electron correlation, rendering them particularly challenging for conventional excited-state methodologies. Standard approaches such as CIS, RPA, and LR-TDDFT fail to accurately capture the singlet-triplet inversion, largely due to the inadequate treatment of double excitations in S_1 [1]. However, the intricate electronic structure of these systems—where S_0, S_1, and T_1 all involve significant contributions from double and higher-order excitations—necessitates a fine balance between static and dynamic correlation for reliable energy predictions. In this work, we undertake a comprehensive investigation of these molecules using a systematically layered hierarchy of single- and multi-reference wavefunction-based methods, alongside density functional theory (DFT) approaches. Our study is driven by three key objectives: (a) unraveling the essential electronic configurations that define the nature of the relevant states, (b) establishing high-fidelity benchmark data for excitation energies, and (c) identifying an efficient yet accurate computational protocol suitable for large-scale screening of more complex derivatives and oligomers. The ultimate goal is to pinpoint practical molecular candidates that exhibit optimal spin-orbit and spin-vibronic interactions, along with favorable ISC and RISC rate constants, for OLED applications. Furthermore, we examine the influence of spin contamination and spin polarization, drawing meaningful connections to minimal two- and three-state exciton models to distill the fundamental physics governing these exotic electronic interactions.

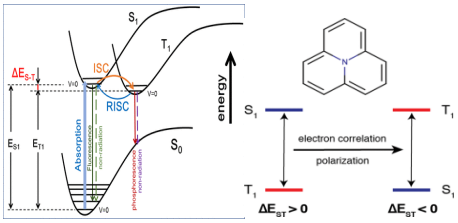


Figure 1: Violation Of Hund's law

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Study of stochastic thermodynamics and dynamic hysteresis in a driven chemical system

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We aim to study the kinetic and thermodynamic aspects of chemical computation. The results of the analyses would provide us with an idea of the advantages and disadvantages of chemical computation as compared to the conventional computational processes. The laws of stochastic thermodynamics guide the speed, accuracy, and efficiency of information processing in computers. The components of the chemical computational processes are reported to be the reaction networks involving autocatalytic steps. Therefore, we focused on a specific chemical reaction network represented by the Schlögl model, where autocatalytic steps are present that lead to the bistability in terms of the concentration of the autocatalytic species involved in the reaction. The external drive is incorporated in the reaction network through the rate of pumping of another species. This pumping is considered to be periodic in time. The process manifests as a stochastic resonance phenomenon, and we study this resonance phenomenon in terms of a very important measure for stochastic resonance, the hysteresis loop area. Hysteresis loops are observed due to the lag between the system's response, here the concentration of the autocatalytic species, and the external periodic drive implemented through the pumping of the product species. We notice the turnover of the quantity with respect to the relevant parameters of the dynamics. We suggest that our present study can be considered to be the initial steps in understanding the kinetic aspects related to chemical computation.

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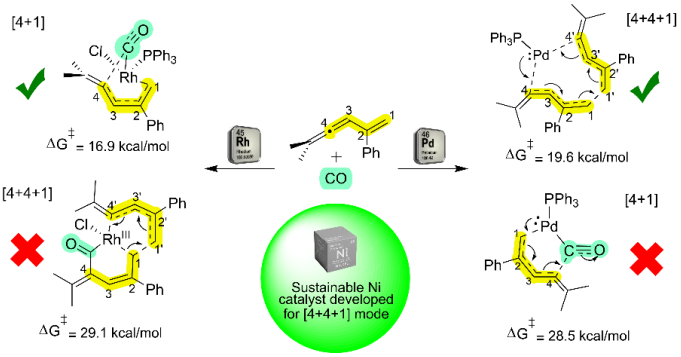
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Why Does Rh Prefer [4 + 1] while Pd Prefer [4 + 4 + 1] Mode in Carbocyclization of Vinylallene with CO? Unveiling Nickel's Potential for Expanding the Scope Beyond Pd

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Rhodium(I) promotes a [4 + 1] assembly mode with a vinylallene substrate and CO, leading to the formation of a five-membered ring structure. In striking contrast, palladium(0) catalyzes a more complex [4 + 4 + 1] mode leading to a nine-membered cyclic ketone. The underlying mechanisms that govern this contrast in assembly modes remain unclear, even in today's date, presenting a major challenge to the further development of efficient reactions. Our computational study[1] reveals that Rh adopts a square pyramidal geometry with CO. This is in contrast to Pd, which prefers a trigonal planar geometry. A stronger metal–CO interaction is detected in Rh than in a Pd intermediate, making the [4 + 1] mode more preferable in Rh than in Pd. The transition state for C–C coupling between two vinylallene has a significantly distorted tetrahedral core in the case of Rh, while Pd retains a stable trigonal planar structure, making the [4 + 4 + 1] reaction less favorable in Rh than in Pd. By conceptualizing and transferring the critical features of Pd to Ni systems, we have rationally designed a Ni-catalyzed [4 + 4 + 1] version that combines the desirable reactivity of Pd with the cost-effectiveness and abundance of Ni, aligning with the growing demand for more sustainable and atom-efficient strategies in synthetic organic chemistry.



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Mechanistic Elucidation of Iron Catalysed Sonogashira Coupling via Density Functional Theory

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The Sonogashira-type cross-coupling reaction represents one of the most versatile and widely utilized strategies for constructing C(sp^2)–C(sp) bonds, a key structural motif in aryl alkynes. These compounds serve as important building blocks in pharmaceuticals, natural products, and functional materials, underscoring the synthetic value of this transformation. Traditionally mediated by palladium catalysts, recent efforts have shifted toward the development of cost-effective and environmentally sustainable alternatives, with iron catalysis emerging as a promising candidate. In this study, the mechanistic underpinnings of the iron-catalyzed Sonogashira-type coupling between phenylacetylene and 4-iodoacetophenone were systematically explored through Density Functional Theory (DFT) calculations. The catalytic system employed $FeCl_3 \cdot 6H_2O$ in conjunction with 1,10-phenanthroline as a ligand, operating in aqueous medium under aerobic conditions. The computational findings highlight a reaction pathway that initiates with base-assisted activation of the terminal alkyne, followed by coordination of the aryl halide to the iron center. The subsequent C–C bond formation is predicted to occur via a concerted mechanism, avoiding discrete radical intermediates. Notably, the entire cycle is redox-neutral, maintaining iron in the +3 oxidation state throughout. These insights not only clarify the role of iron in promoting selective bond construction but also provide a theoretical foundation for advancing green, sustainable and non-precious metal cross-coupling methodologies.

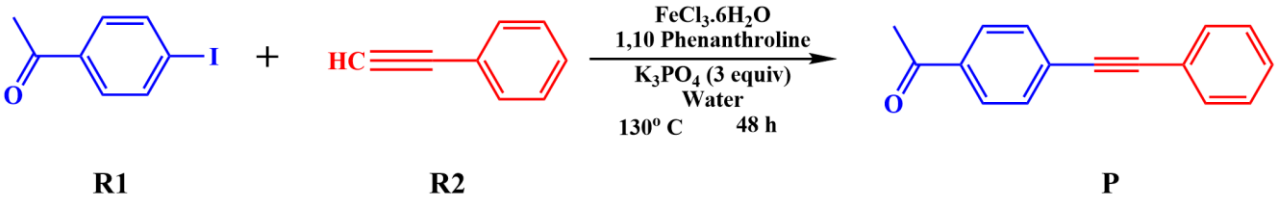


Figure 1 Iron-Catalyzed Sonogashira Coupling between 4-iodoacetophenone and phenylacetylene

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FeC_4H_2: A Potential Astrophysical Molecule Featuring Planar Tetracoordinate Iron to Unveil the Mystery of Missing Iron in Interstellar Medium

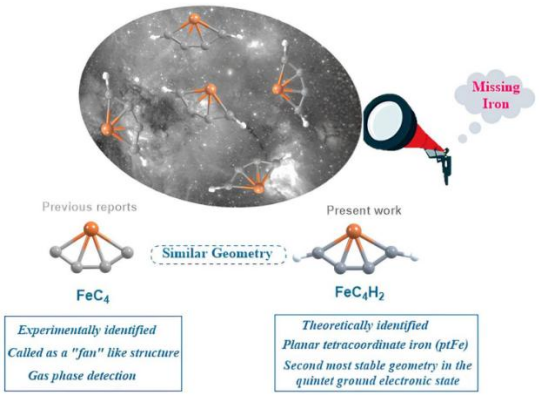
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The exploration of iron-containing species represents a prominent area in contemporary astrochemical investigations. Iron in the interstellar medium exhibits predominantly low concentrations, hinting at the potential presence of missing iron in either a condensed or molecular state. The FeC_4H_2 neutral system has been investigated using computational calculations, emphasizing the hypothesis that missing iron may exist as iron−carbon hydride compounds or their higher order. A total of 61, 46, and 36 stationary points have been identified on the potential energy surface (PES) of the FeC_4H_2 in the singlet, triplet, and quintet electronic states, respectively, showcasing the existence of a planar tetracoordinate iron (ptFe). A linear geometry represents the global minimum on the PES of FeC_4H_2 as observed in the quintet ground electronic state. Meanwhile, the ptFe geometry is identified as the second most stable isomer in the quintet electronic state, which is the lowest energy solely in the singlet electronic state. Further, the observed ptFe geometry closely resembles the experimentally detected FeC_4 molecule in the gas phase. In light of its similarity to FeC_4 and the recent detection of FeC in the interstellar medium, the ptFe would be a potential astrophysical molecule that will also be identified in the gas phase. From that point of view, a comprehensive examination of the nature of chemical bonding of the ptFe geometry in the singlet, triplet, and quintet electronic states has been characterized, which dictates the stabilization of ptFe through multicenter bonding with surrounding carbon atoms. Ab initio molecular dynamics simulations revealed the dynamic stability of the system. Understanding the interstellar species with its structure and chemical bonding is an important aspect that would shed light on new insights into the experimental observations in the future.



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Crowding Effects on Structural Preferences of Amyloid Oligomers

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Abstract:
Understanding protein folding and aggregation requires incorporating the effects of crowded *in vivo* environments, where excluded volume effects and soft, non-specific interactions can strongly influence the hydration and biomolecular processes. Intrinsically disordered proteins (IDPs), such as amyloid-β (Aβ) and α-synuclein, are a special class of proteins with disordered regions that can misfold and assemble into highly ordered aggregates called amyloid fibrils. They play a key role in neurodegenerative diseases and are strongly influenced by *in vivo* conditions. Using molecular dynamics simulations, we investigated the stability of Aβ(16–22) dimers and tetramers in the presence of molecular crowders such as ethylene glycol (EG), diethylene glycol (DEG), and a hydrophobic variant of DEG (UCON) at various packing fractions. Our results show that EG destabilizes peptide oligomers by enhancing hydration at low packing fraction and peptide–crowder interactions at high packing fraction. In contrast, UCON stabilizes oligomers via two mechanisms: at low concentrations by reducing hydration water around oligomers and increasing inter-peptide interactions, and at high concentrations through entropic volume exclusion that confines hydration water around the peptides. Confined water is found to be disordered with anomalously slow diffusion, highlighting its key role in modulating oligomer stability.[1] We further extended our work to investigate how the structural stability of amyloid oligomers of α-synuclein is affected in the presence of macromolecular crowders modelled by PEG600. The role of crowder conformational flexibility on the structural preferences of amyloid oligomers was investigated. These studies bridge molecular and macromolecular crowding regimes, providing a unified view of how crowded environments regulate protein free energy landscapes.

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Anisotropic Pair Potentials Involving Aromatic Hydrocarbons: Aggregate Geometries via Swarm Intelligence Approach

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Intermolecular interactions between aromatic hydrocarbons have been extensively studied in recent years using electronic structure theory methods[1-3]. However, such computations for large clusters using electronic structure theory methods are computationally expensive, and their applicability is generally limited to the case of dimers. In contrast, large aromatic hydrocarbon clusters have been investigated using computationally efficient empirical potentials[4]. Moreover, modeling interactions between aromatic hydrocarbon aggregates with appropriately parametrized potentials efficiently captures the energy landscape, while consuming much less computational time.

In aromatic hydrocarbon systems, accurately capturing subtle variations in interaction energetics and preferred geometries across different configurations is essential. The isotropic pair potentials offer limited scope for capturing such subtleties. Therefore, in this work, we model the intermolecular interactions using three empirical potentials: the Lennard-Jones potential, which is isotropic in nature, and two different variations of the Carlos and Cole (CC) potential[5], which captures the anisotropy in interatomic interactions. The first variant (CC-I) introduces anisotropy only in the short-range repulsive interactions, whereas the second variant (CC-II) incorporates anisotropy in both the short-range repulsive and long-range attractive terms. All the three potentials were parametrized using reference data obtained from dispersion-corrected density functional theory (B3LYP-D3BJ/6-311++G(d,p)) calculations. The resulting parameter sets were validated by assessing their transferability across different dimer configurations and other aromatic hydrocarbon systems. Among the potentials considered, the CC-II potential was most effective in capturing anisotropic interaction characteristics within the aggregates. To compute the minimum energy configurations of the aromatic hydrocarbon clusters, we used a stochastic optimization strategy known as the particle swarm optimization (PSO)[6] in conjunction with the parametrized CC-II potential[7,8].

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Automated Digital Design of Homogeneous Catalysts

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Identifying molecular catalysts that achieve a balance of high selectivity and rapid reaction rates presents a significant challenge in modern homogeneous catalysis. The traditional approach to catalyst discovery—relying on extensive and costly trial-and-error experimentation—is inefficient and slow. Here, we introduce the *insilico* modeling approach based on Physics- and AI-based design of homogeneous catalysts to rapidly screen, predict, and optimize the performance of potential molecular catalysts, as implemented in Schrodinger Material Suite.**[1]**

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Thermophysical properties of metallic melts through microscopic structural functions.

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This study provides a theoretical analysis of the structure, thermodynamics and acoustic properties of ten liquid metals using the Square Well (SW) model. The computed results for the static structure factor, $S(k)$ and radial distribution function, $g(r)$, of three liquid metals have been compared with available experimental results. The long wavelength limit of the static structure factor, $S(0)$, is linked to a thermo-physical property, i.e. adiabatic compressibility factor, β_S through the relation $S(0) = \rho K_B T \gamma \beta_S$ which is obtained from the SW equation of state. The adiabatic compressibility factor is then used to evaluate the sound velocity of metallic melts.

Table 1 Computed thermophysical properties of metallic melts.

Metals	Temp.(K)	S(0)	$\beta_S \times 10^{-10}$(m^2/N)	v_s(m/s)
Li	463	0.0230	0.89	4725
Na	378	0.0253	1.78	2440
Al	943	0.0164	0.15	4550
K	343	0.0245	3.68	1810
Cu	1423	0.0291	0.16	2965
Zn	723	0.0169	0.23	2746
Rb	313	0.0342	6.99	1036
Ag	1273	0.0229	0.18	2549
Cs	303	0.0233	5.80	960
Au	1373	0.0160	0.13	2182

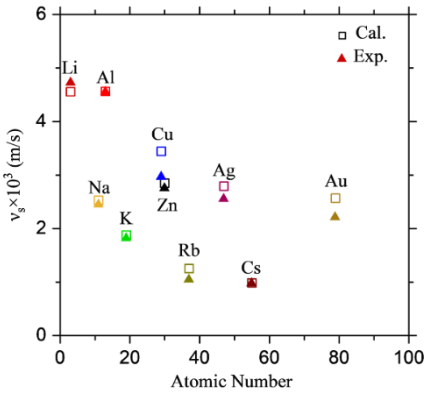


Figure 1 Theoretical and experimental values of sound velocity of liquid metals vs atomic number.

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Multireference Density Matrix Embedding Theory for Molecules and Defects

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Quantum embedding methods have emerged as powerful tools for electronic properties in systems with strong electron correlation[1]. In this work, we employ Density Matrix Embedding Theory (DMET) in conjunction with complete active space self-consistent field (CASSCF), n-electron valence state perturbation theory (NEVPT2), and multiconfigurational pair density functional theory (MC-PDFT) to study both molecular and periodic systems exhibiting localized multireference character. For extended transition metal complexes, density matrix embedded PDFT (DME-PDFT)[2], provides a substantial cost reduction compared to traditional nonembedded MC-PDFT. We have validated the method by computing the bond dissociation in methyl diazine and spin-splitting energy gap in the $[Fe(H2O)_6]^{2+}$ complex, showing that DME-PDFT splitting energies converge faster compared to NEVPT2-DMET to the corresponding nonembedding limits. We finally compare embedding schemes with truncation schemes for two extended transition metal complexes, Fe[N(H)Ar*]2 and $[NiC_{90}N_{20}H_{120}]^{2+}$, and show that embedding schemes are more accurate than truncations when the transition metal is not fully coordinated.

For defects in periodic systems, we investigate the F0 color center in bulk MgO, where the nature of the optically active states remains debated. To estimate defect-localized vertical excitation energies at the nonembedding and thermodynamic limits, a double extrapolation scheme is employed[3]. The extrapolated NEVPT2-DMET vertical excitation energy value of 5.24 eV agrees well with the experimental absorption maxima at 5.03 eV, whereas the excitation energy value of 2.89 eV at the relaxed triplet defect-localized state geometry overestimates the experimental emission at 2.4 eV by only nearly 0.5 eV, indicating the involvement of the triplet–singlet decay pathway.

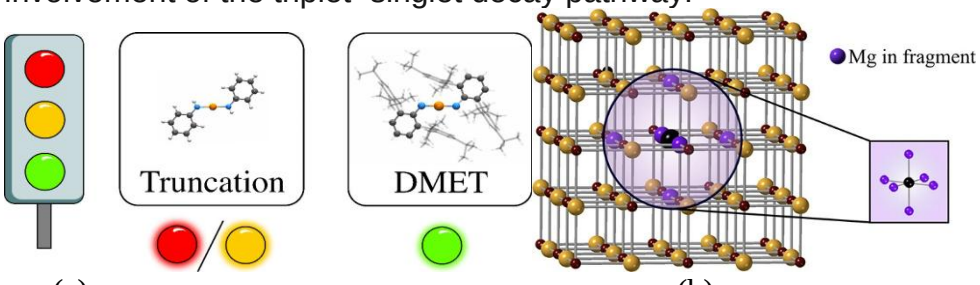


Figure 1: (a) A truncated-ligand model for the Fe complex, and the full complex with the DMET fragment atoms highlighted. (b) Cubic MgO crystal with the DMET fragment cluster ($OV–Mg_6$) consisting of the nearest-neighbour 6 Mg atoms around the oxygen vacancy.

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Computational insights into Modulating the Magnetic Anisotropy in Co(II)/Dy(III) based Single Molecule Magnets

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Several advances have been made in the field of single molecule magnets (SMMs) with the aim of enhancing their magnetic anisotropy to allow for slow relaxation of magnetisation. Structural distortions, particularly in transition metal and lanthanide based mononuclear complexes, have been found to significantly influence magnetic anisotropy. Another key strategy involves introducing heavy atoms into the ligand environment to enhance spin-orbit coupling and metal-ligand covalency.[1–4] My first work examines Co(II) tetrahedral complexes using ab-initio methods to evaluate the effects of ligand modifications on magnetic anisotropy. We vary the donor atom from nitrogen to bismuth in $Co(ER_2)I_2$ molecules and investigate structural distortions using $[Co(pdms)_2]^{2-}$ motif with varying bite angles of the ligand. The second work explores Dy(III)-based unsaturated 18C6 crown complexes in hexagonal bipyramidal environments. We study $[C_{12}H_{12}E_6]$ (E = O, S, Se) rings as equatorial ligands and halides (F, Cl, Br, I) as axial ligands. These investigations provide insights into design principles towards enhancing the magnetic anisotropy in next-generation SMMs.[5,6]

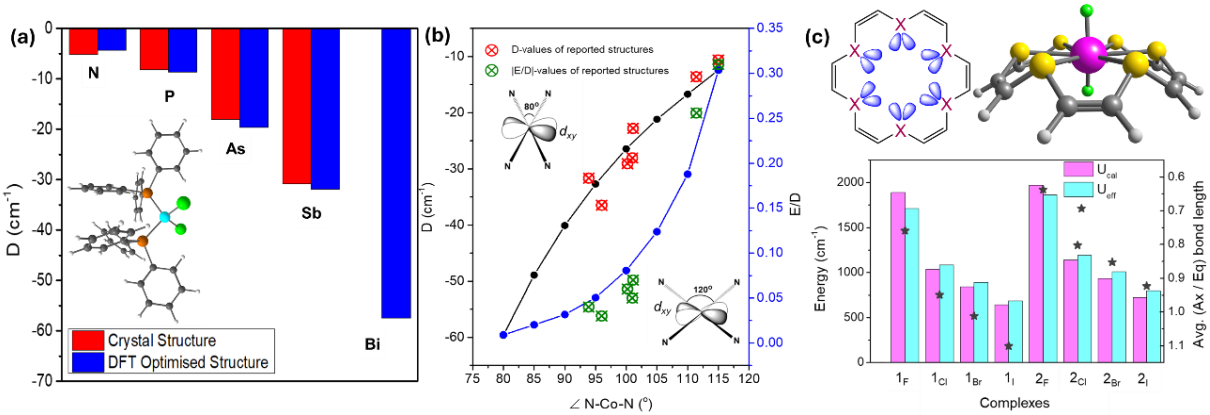


Figure 1: (a) Variation in D-value with inclusion of heavy atom in Co(II) complexes; (b) Correlation between the bite angle and the D-value; (c) Effect of ligand modulation in hexagonal bipyramidal Dy(III) complexes

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Quantum Thermal Logic Gates

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We propose a novel framework for *Quantum Thermal Logic Gates (QTLGs)* [1], serving as the thermal analog of conventional electronic logic gates, where logical operations are carried out using heat currents instead of charge currents. Specifically, we demonstrate that a double quantum-dot junction [2,3], coupled to electronic thermal reservoirs, can effectively implement fundamental logic operations in a quantum circuit [1,4]. By carefully tuning the system parameters, we establish a clear one-to-one correspondence between various operational modes of classical electronic logic gates and their quantum thermal counterparts. Furthermore, we outline a feasible experimental setup [1,5], highlighting a potential nano-electronic circuit architecture for realizing QTLG-based computation. Our results suggest a promising route toward integrating thermal transport phenomena into future quantum information processing and nano-electronic device technologies.

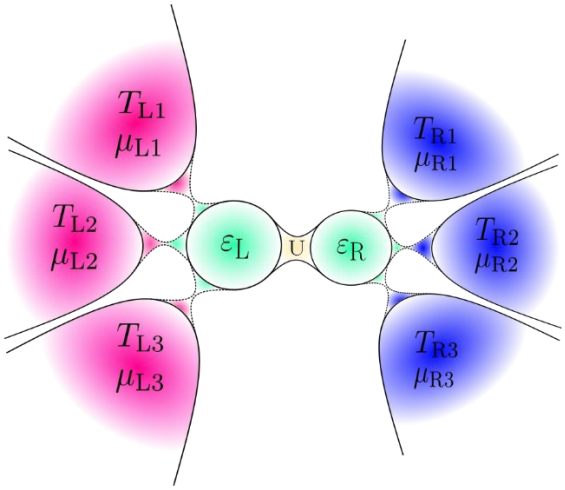


Figure 1 Schematic of two strongly Coulomb-coupled quantum dots (QDs) located at the center, with their single-particle energy levels denoted by $\boldsymbol{\varepsilon_L}$ and $\boldsymbol{\varepsilon_R}$, and the interdot interaction strength by $\boldsymbol{U}$. Each dot is weakly coupled to one or more fermionic leads that serve as thermal-logic input and output terminals. The left (right) leads are characterized by their temperature $\boldsymbol{T_L}$ ($\boldsymbol{T_R}$) and chemical potential $\boldsymbol{\mu_L}$ ($\boldsymbol{\mu_R}$), respectively, thereby enabling heat-current–driven logic operations.

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Theoretical Elucidation of Photoelectron Spectrum of Diphosphatriazolate Anion, $P_2N_3^-$

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In this study, the 193 nm photoelectron spectrum of P_2N_3 is analyzed using comprehensive *ab initio* electronic structure and quantum dynamics computations, with a focus on the first five low-lying electronic states (X, $\tilde{A}$, $\tilde{B}$, $\tilde{C}$, and $\tilde{D}$) of P_2N_3. A 5 × 5 model Hamiltonian is constructed within a diabatic electronic framework to facilitate time-dependent (TD) and time-independent (TI) quantum chemical calculations. Nonadiabatic effects arise from energetically close electronic states possessing multiple crossings and conical intersections within them. The experimental photoelectron spectrum is thoroughly interpreted, accounting for all of the observed peaks and proper vibronic assignments. Notably, the first peak corresponds to four electronic states X, $\tilde{A}$, $\tilde{B}$ and $\tilde{C}$, while the second peak is attributed to the $\tilde{D}$ state of P_2N_3. Overall, our theoretical model deduced spectra coincide satisfactorily with the experimental results.

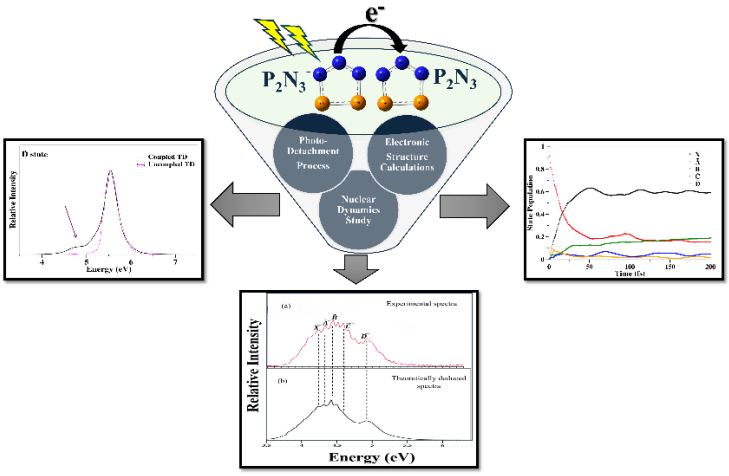


Figure 1 Pictorial diagramme of rationalizing exprimenal photoelectron spectra of P_2N_3 using vibronic coupling theory.

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Computational Insights into Iron-Iodine Catalyzed Hantzsch Condensation:A Route to 2-Aminothiazoles

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2-aminothiazoles are crucial class of heterocyclic compounds in pharmaceutical research, and are known for their wide spectrum of biological activities.This work aims to elucidate the mechanism of the Iron-Iodine Catalyzed Hantzsch type condensation,which provides a highly efficient pathway for the synthesis of these important heterocycles, Where a cost-effective and easily available catalytic system comprising $FeCl_3.6H_2O$ and Molecular Iodine. The methodology enables the synthesis of various 2-Aminothiazoles with moderate to high yields. All the calculations were performed using Density Functional Theory [DFT] level at the B3LYP functional with Grimme's D3 dispersion corrections, providing a framework. Conductor like Polarizable Continuum Model(CPCM)solvation model with PEG-400 as the solvent was used to account for solvation effects.The Plausible mechanistic pathway is being investigated and likely intermediates are identified and optimized. This work makes notable contribution to the field by presenting a convenient and feasible method for synthesizing biologically important 2-Aminopyridines ,with promising implications for drug discovery and development. The work illuminates the importance of having theoretical background by providing a deeper understanding of the reaction pathways for organic synthesis reactions.

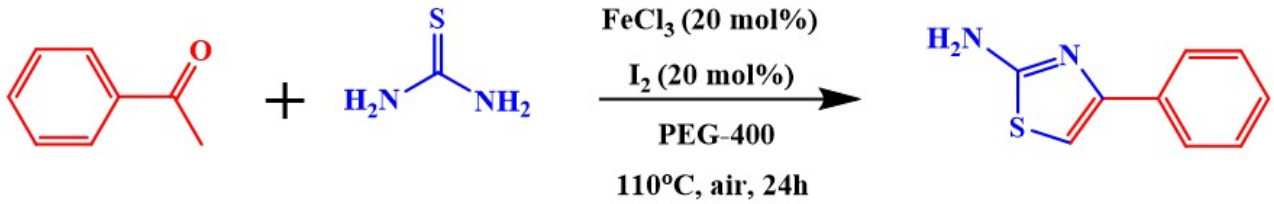


Figure 1 Iron-Iodine Catalyzed Hantzsch type Condensation

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"MTASpec Software for Ab Initio Spectroscopic Calculations of Large Molecules"

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Spectroscopic methods, including infrared (IR), Raman, vibrational circular dichroism (VCD), Raman optical activity (ROA), and nuclear magnetic resonance (NMR), are essential for elucidating molecular structure and its chirality. These techniques are important for conformational analysis and structural determination. The recently developed MTASpec software, based on the Molecular Tailoring Approach (MTA), offers an efficient and scalable framework for ab initio computation of vibrational spectra, including IR and Raman. MTASpec automates the fragmentation of substantial molecules into overlapping segments, compute quantum chemical computations on individual fragment, and rebuilds global molecular properties with near-complete accuracy compared to full molecule calculation with significantly diminishing memory requirements and computational time. Based on this framework, MTA has been further extended this year to evaluate chiroptical responses (VCD and ROA) and NMR characteristics such as isotropic shielding and spin-spin coupling constants. This unified technique allows for precise ab initio treatment of both vibrational and magnetic resonance spectroscopies while remaining computationally efficient. MTASpec is intended for widespread use and will soon be available online with MTASpec2.0, allowing researchers worldwide to undertake high-accuracy spectroscopic simulations of huge systems using little computer resources. Overall, the combination of MTASpec and MTA offers a potent and cost-effective approach to scalable theoretical spectroscopy across several analytical techniques.

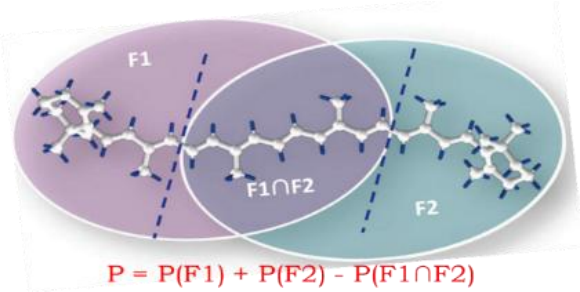


Figure 1. Molecular fragment used in MTA

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Water Absorption Free Energy in Biochar Models using Thermodynamic Integration

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Biochar, a well-known carbon compound produced through the thermal decomposition (pyrolysis) of biomass under oxygen-limiting environments [1], has shown a promising role in carbon sequestration and soil amendments to improve its fertility. Not only the soil but also biochar is widely used for wastewater treatment and air pollutant removal, which makes it the most environmentally friendly material for sustainability. One important aspect of using biochar as a soil amendment is its ability to enhance the water retention capacity of the soil [2]. Present work focuses on the in-silico study of the water absorption mechanism of biochar produced at different pyrolysis temperatures. Wood et al. [3] biochar models, constructed at various pyrolysis temperatures, were used to generate biochar surface-water interfaces to understand the water absorption using molecular dynamics simulations. The Thermodynamic Integration (TI) method was employed to obtain the absorption free energy (ΔG) for all the models. Solvent accessible surface area (SASA) and absorption free energy illustrate that the water absorption capacity of biochar varies significantly with pyrolysis temperature.

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Mechanistic Insights into Zirconocene-Catalyzed Ethylene/1-Octene Copolymerization: Kinetic Hindrance Governs α-Olefin Insertion

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Olefin polymerization using single-site metallocene catalysts,[1] like zirconocenes, is vital for producing high-performance polyolefins. While these catalysts effectively control polymer properties, achieving high comonomer incorporation—specifically of higher α-olefins like 1-octene alongside ethylene—remains a significant challenge. This computational study employs density functional theory (DFT) to perform a mechanistic investigation of the copolymerization of ethylene and 1-octene using a modified zirconocene catalyst, rac-dimethyl silyl bis(1-indenyl) zirconium dichloride, aiming to identify factors that control comonomer incorporation (Figure 1). DFT calculations, performed with and without a counteranion (BARF and MAO)[2] and across different implicit solvents, consistently showed that higher olefins (1-butene, 1-hexene, 1-octene) have a thermodynamic preference for initial π-complex formation with the catalyst compared to ethylene (ΔG is more negative). However, this initial advantage was overridden by kinetics: the subsequent insertion step for ethylene proceeds through a significantly lower kinetic barrier than for the higher olefins. Further analysis of the β-hydrogen agostic interaction, uptake barrier and rotational barriers supported the finding that higher analogues of ethylene (α-olefin) insertion faces greater kinetic hindrance.The results unequivocally demonstrate that the insertion barrier is the primary factor dictating the final product composition, favoring the polymerization of ethylene. A reduction in the insertion barrier for α-olefins is crucial for achieving improved comonomer incorporation. These insights will guide the rational design of novel Zr metallocene catalysts for enhanced comonomer insertion.

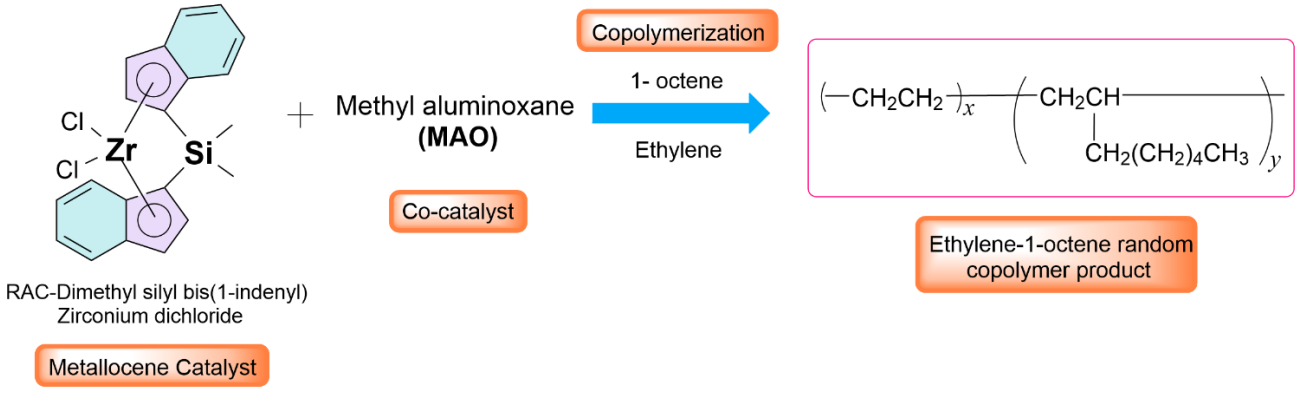


Figure 1 Homogeneous Copolymerization of Ethylene and 1-Octene.

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A Computational Study on cis–trans Photo and Thermal isomerizations of Azobis(benzo-15-crown-5) and its Metal Ion Complexes

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Computational studies on the thermal and photo-induced cis-trans isomerizations of photoresponsive azobis(benzo-15-crown-5) have been carried out (Figure 1). For the trans isomer, the photoexcited ππ* (S_2) state relaxes via a planar minimum and a planar S_2/S_1 conical intersection along the N═N stretching coordinate, while the nπ* (S_1) state features both planar and rotational minima, where the latter leads to a torsional S_0/S_1 conical intersection with a CNNC dihedral angle value close to 90°. The rotational pathway exhibits an energy barrier which is lowered through a coupled N–N out-of-plane motion, facilitating the trans→cis isomerization. In contrast, the cis isomer undergoes barrierless photoisomerization along the S_1 surface via a torsional S_0/S_1 conical intersection, where as the S_2/S_1 CI lies too high in energy to be accessed upon ππ* excitation. Thermal cis → trans thermal isomerization proceeds through an inversion pathway forming a less stable trans form. The rotational counter part of this pathway requires more barrier, however, along this route a non-adiabatic singlet-triplet (S_0/T_1) crossing has been noticed which opens a comparatively easier cis→trans conversion pathway. In recent times, we have performed alkali metal-initiated isomerization processes of this crown ether which is related to the ion transport phenomenon. Presence of counter anion is found to influence these isomerizations as it eases the opening of the cis form which subsequently undergoes a conical intersection (S_0/S_1) to form the trans isomer.

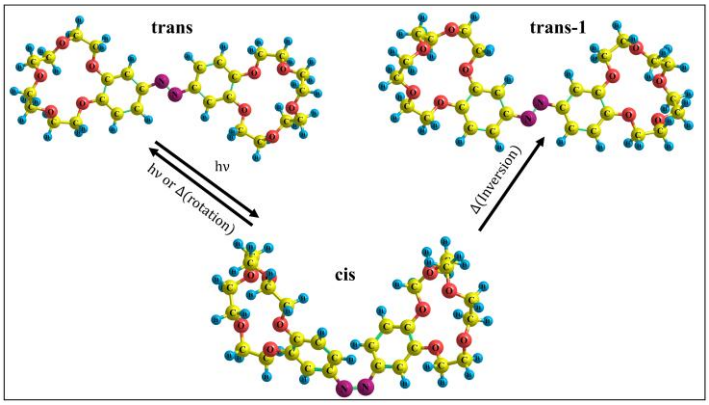
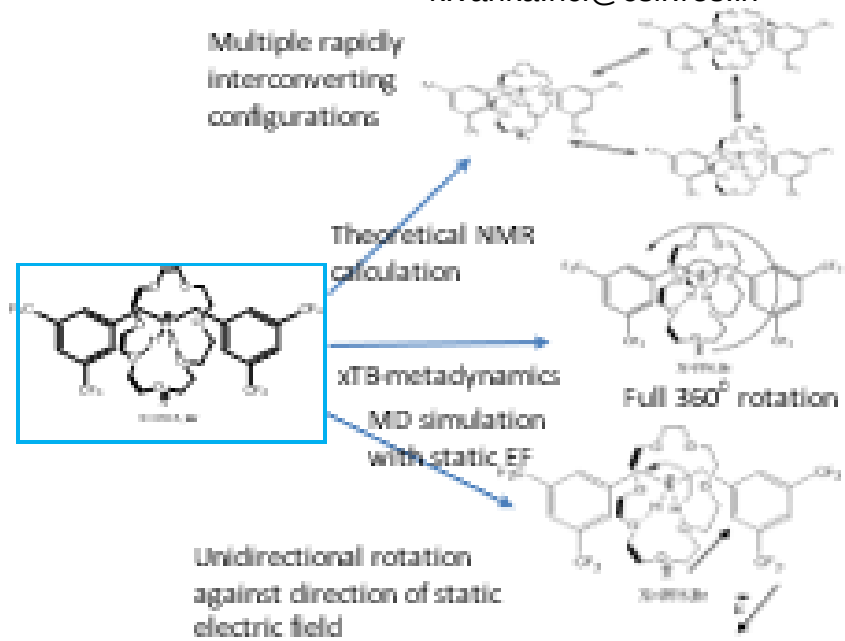


Figure 1. Thermal and photo-induced isomerizations of photoresponsive azobis(benzo-15-crown-5)

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Computational Study reveals that full rotational motion of the Compact Superbases Rotaxane

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DFT studies and MD simulation indicates that compact superbase rotaxane shows complete unidirectional rotational motion in the presence of the electric field and thereby we predicts it can acts as molecular motor in presence of the external electric field.

Figure 1 - The different methods used to prove the potential of compound for molecular motor

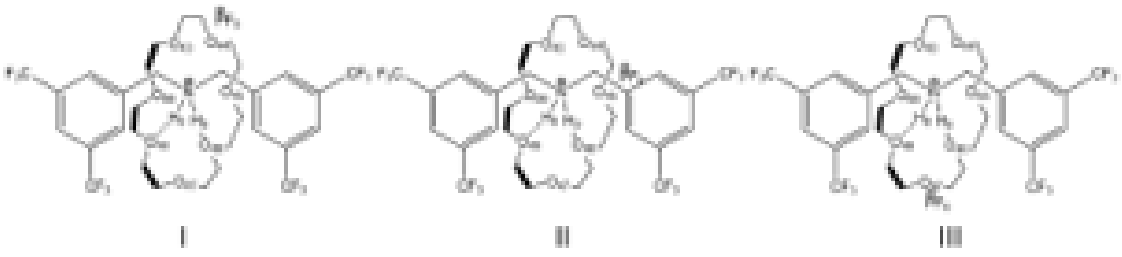


Figure2-NMR calculated structure of the rotaxane at three different position ie, RFS- (one in back, side and front position w.r.t NH2 moiety (I, II & III respectively)

Table 1-Comparison of the Theoretical NMR value of the two hydrogen with experimental value of three configuration ie, RFS- (one in back, side and front position w.r.t NH2 moiety (I, II & III respectively)

NMR calc at TPSSTPSS-d3/tzvp/CPCM(MeCN)					
TPSSTPSS/tzvp/ CPCM(MeCN)	I	II	III	Average	Expt. [1]
H8	8.27	7.86	8.44	8.19	8.00
H9	7.75	8.05	8.57	8.12	8.00

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In Silico Study of Disruption of Amyloid-Beta Mature Fibril by the Silent Allosteric Modulator BMS-984923

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Amyloid aggregation is a key pathological hallmark of Alzheimer's disease (AD). According to clinical studies, abnormal self-aggregation of Amyloid-beta peptide into toxic oligomeric species which subsequently form fibrillar aggregates is linked to the development of AD. Therapeutic strategies targeting this aggregation include stabilization of the monomeric Amyloid-beta, or destabilization of the mature fibrils. BMS-984923, a silent allosteric modulator of metabotropic glutamate receptor 5 (mGluR5), binds without disrupting normal glutamate signaling and has shown efficacy in an AD mouse model (APPswe/PS1ΔE9) by preventing Aβ oligomer-induced toxicity, rescuing memory function, and reducing synaptic loss. However, the molecular mechanism remains elusive. In this study, molecular docking and molecular dynamics (MD) simulations are performed using the Aβ fibril structure (PDB ID: 2BEG). Docking revealed favorable initial binding free energy of –8.61 kcal/mol with BMS-984923 interacting primarily with residues in chains A (1–26) and B (27–52). MD simulations showed increased RMSD, RMSF, radius of gyration (RoG) and SASA values in the ligand-bound system, indicating fibril destabilization. MM/PBSA analysis yielded a binding free energy of –32.57 ± 3.64 kcal/mol, and per-residue energy decomposition identified key contributions from chains D and E. Secondary structure analysis using DSSP showed a reduction in β-sheet content from 45.20% (ligand-free) to 37.20% (ligand-bound), supporting the compound's destabilizing effect. Free energy landscape (FEL) analysis further indicated that the ligand-bound system sampled fewer, lower-energy conformational states compared to the ligand-free fibril. These results provide mechanistic insights into how BMS-984923 disrupts Aβ fibril stability, supporting its potential as a therapeutic agent in AD.

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Mechanistic Pathways of Zinc-Catalysed Clauson–Kaas Reaction: A Density Functional Theory Approach

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Pyrroles, five-membered heterocyclic compounds containing nitrogen as the heteroatom, play a crucial role in pharmaceuticals, agrochemicals, and related fields. The Clauson–Kaas reaction has emerged as a powerful method for synthesizing N-substituted pyrroles, with recent studies focusing on the use of zinc-based catalysts. Although several experimental investigations of zinc-catalysed Clauson–Kaas reactions have been reported, their mechanistic pathways remain poorly understood. Here, we present a density functional theory (DFT) study on the mechanism of a zinc triflate–catalysed Clauson–Kaas reaction under neat conditions. This approach provides cost-effective and eco-friendly access to N-substituted pyrroles (Afsina et al., 2022). All calculations were carried out at the B3LYP level, employing the LANL2DZ basis set for zinc and the 6-31+G(d) basis set for all other atoms. Our proposed mechanism indicates that zinc triflate itself acts as the active catalyst. The reaction begins with coordination of zinc triflate to tetrahydrofuran, followed by nucleophilic attack of a primary amine. These findings offer valuable theoretical insights into the molecular-level mechanism of zinc-catalysed Clauson–Kaas reactions and can guide the design of more efficient catalysts and reaction conditions for future experimental studies.

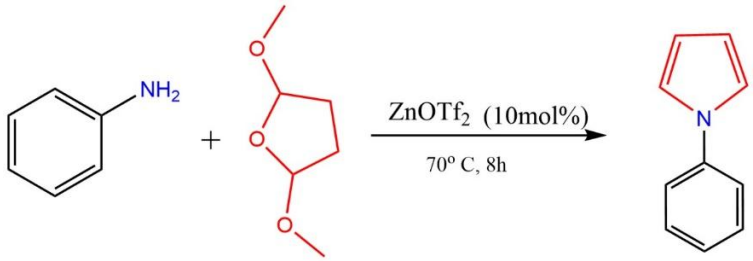


Figure 1 Model system: Zn- catalyzed Clauson Kaas reaction between 2,4-dimethoxy tetrahydrofuran and aniline synthesising N-substituted Pyrroles

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How Hydricity Dictates the Critical Steps of Base-Promoted CO_2 Hydrogenation Reactions?

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Transition metal-catalyzed homogeneous hydrogenation of CO_2 to formate or formic acid has emerged as an attractive method for converting CO_2 into value-added chemicals. Since the state-of-the-art catalysts in this realm are primarily based on expensive precious metals and require demanding reaction conditions, the design and development of economically viable non-noble metal catalysts are in great demand. Herein, we establish the correlation between the thermodynamic hydricity($\Delta G^{\circ}_{H^-}$) and critical reaction steps involved in the correlation between the crucial reaction steps of CO_2 hydrogenation, that is, base-promoted H_2-splitting and hydride transfer to CO_2. A set of three non-noble metal complexes, one bearing tri-coordinated PNP-pincer (**1$_{Mn}$**) and the other two based on tetra-coordinated PNPN-pincer (**2$_{Mn}$** and **3$_{Fe}$**), has been investigated in this study. The computational mechanistic investigation establishes the role of the "internal" amine base in heterolytically splitting the metal-bound H_2. Furthermore, the correlation between the hydricity ($\Delta G^{\circ}_{H^-}$) of *in situ* generated metal-hydride species and the free energy barrier of the two crucial steps could provide an optimal hydricity value for efficient catalytic activity. Overall, this study demonstrates how the crucial thermodynamic and kinetic parameters for pincer-based complexes possessing an "internal base" can be correlated for the prediction of novel non-noble metal-based catalysts for CO_2 hydrogenation. Finally, how hydricity controls the crucial reaction pathway is also being investigated with metal-pincer complexes.

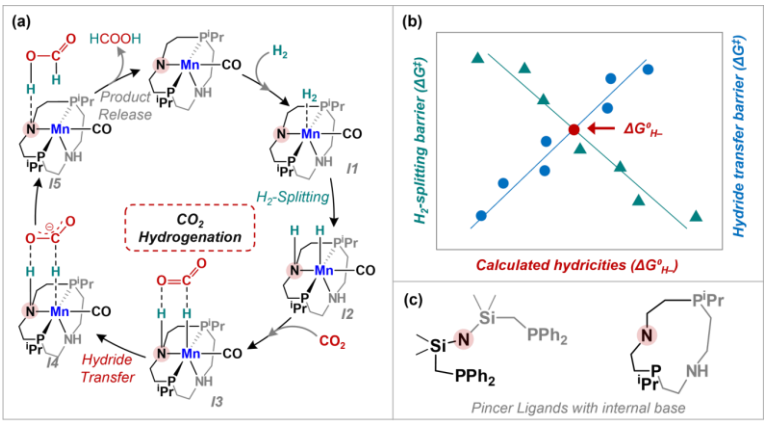


Figure 1: (**a**) Established reaction mechanism and steps involved in homogeneous CO_2 hydrogenation. (**b**) Schematic representation of the correlation diagram between the two key reaction steps of CO_2 hydrogenation and hydricity. (**c**) Chemical structures of the tri- and tetra-coordinated pincer ligands.

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Theoretical Chemistry Symposium
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Correlating Ligand Properties with Photocatalytic Efficiency

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Accurately predicting photocatalytic efficiency in ligand-functionalized metal nanoparticles (NPs) requires a fundamental understanding of interfacial charge transfer dynamics. We present a computational framework integrating Marcus-Hush theory with density functional theory (DFT)-derived parameters—including electronic coupling matrix elements and orbital energetics—to quantitatively describe electron and hole transfer rates in plasmonic photocatalytic systems[1]. Applying this approach to a class of para-substituted aromatic thiol-functionalized Au NPs for water splitting reveals a strong correlation between theoretically calculated electron transfer rates and experimentally measured hydrogen evolution rates[2]. Comparative analysis of selenol-functionalized NPs demonstrates moderately reduced activity relative to thiol analogues. In contrast, para-hydroxy thiol modification exhibits the highest hole transfer rates, consistent with its superior photocatalytic performance. Systematic parameter analysis reveals that while individual electronic parameters show limited correlation with activity trends, their synergistic integration provides robust predictive capability. This framework establishes a quantitative structure-activity relationship for photocatalytic performance, enabling rational design and screening of ligand-modified metal NP catalysts.

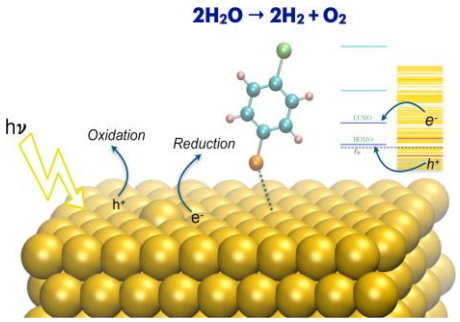


Figure 1: Thiols attached to a gold surface enhance the water splitting reaction.

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UniGEN-DDI: Computing drug-drug interactions using a unified graph embedding network

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Identifying drug–drug interactions (DDIs) is essential for patient safety and treatment efficacy. While some drug combinations yield synergistic benefits, others may cause severe adverse effects, including lethality. Experimental studies provide valuable insights into DDIs but are constrained by cost and time. To address this, we developed UniGEN-DDI (Unified Graph Embedding Network for Drug–Drug Interaction), a computational model for DDI estimation. UniGEN-DDI integrates biochemical association data from DrugBank 5.1.0 and applies a combination of GraphSAGE and Node2Vec to capture diverse drug features efficiently. The model's simple yet unified design reduces computational overhead while achieving high predictive accuracy. Evaluations on balanced datasets and challenging non-overlapping splits based on drug action demonstrated both robustness and efficiency. Notably, UniGEN-DDI identified 15 previously unknown DDIs in the top 20 predictions (75% accuracy) and correctly detected 68% of unknown DDIs among the top 50 predictions, later confirmed by experimental evidence in DrugBank 6.0.

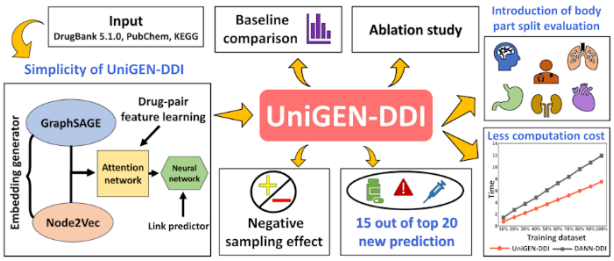


Figure 1 Summary of UniGEN-DDI.

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Theoretical Chemistry Symposium
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Quantum Metrology of Noise Induced Coherences in Systems Out of Thermal Equilibrium

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Abstract

A four level non equilibrium system model with two degenerate ground states $|1\rangle$, $|2\rangle$ and two excited states $|a\rangle$ and $|b\rangle$ is considered in cold alkali atoms coupled with hot (T_h) and cold thermal baths (T_c) and a cavity mode. Coherence defined as existence of the system in superposition states, arises between these two degenerate ground states due to interactions with the hot and the cold thermal baths. Coherence leads to interference between these two states $|1\rangle$ and $|2\rangle$, leading to their hybridization, forming a new hybrid state $|12\rangle$. This hybrid state results in a coherence term ρ_{12} between the states $|1\rangle$ and $|2\rangle$, which can couple to population of states through transitions involving intermediate states like $|a\rangle$ or $|b\rangle$. The strength of this coherence-population coupling depends on the relative orientation of the transition dipole vectors μ_{1a} and μ_{2a} for transitions between states $|a\rangle\leftrightarrow|1\rangle$ and $|a\rangle\leftrightarrow|2\rangle$. This coupling is zero when the transition dipole vectors are perpendicular and maximum when they are parallel. To quantify these effects, two dimensionless parameters p_h and p_c are introduced, representing the relative transition orientation for the hot and cold baths respectively. Estimation of these parameters p_h and p_c are important because quantum coherences can control transition rates between energy levels, allowing control over population dynamics. Measurement of these parameters is experimentally challenging. To estimate these parameters Quantum Fischer information (QFI) computed from the density matrix is used. The QFI tells how precisely a parameter can be estimated embedded in the quantum state of a system. The QFI is defined via the symmetric logarithmic derivative (SLD). Once SLD is calculated, QFI is estimated by taking the trace of the product of the quantum state and the square of the SLD operator.

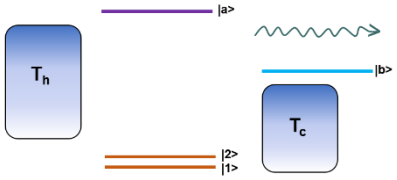


Figure 1. Schematic representation of four level non equilibrium model with degenerate levels $|1\rangle$ and $|2\rangle$ resonantly coupled to excited states $|a\rangle$ and $|b\rangle$ by two thermal baths with temperatures T_h (hot) and T_c (cold). Excited states $|a\rangle$ and $|b\rangle$ are coupled through a cavity mode.

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Beyond DCD: Electron-sharing in Transition Metal-Ligand Complexes

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The Dewar–Chatt–Duncanson (DCD) model[1] has long served as the conceptual foundation for understanding transition metal–ligand bonding, particularly in olefin complexes. However, emerging studies on unconventional ligands such as arynes, fullerenes (C60), and *o*-carborenes[2] reveal significant deviations from this classical framework. Using a combination of NBO[3], QTAIM[4], and EDA-NOCV analysis[5], we systematically investigated bonding interactions across representative transition metal complexes with these ligands. Our results demonstrate that, while a limited subset of late transition metals (e.g., Fe, Ir, Pd, Pt) exhibit bonding consistent with the DCD model, the majority adopt a mixed dative-plus-electron-sharing (D+E) paradigm. In these cases, bonding is best described between electronically charged fragments (TM^+ and $ligand^-$), characterised by dominant electrostatic stabilisation and significant π-electron sharing, with σ-donation playing a lesser role. Collectively, these findings not only highlight the limitations of the classical DCD model but also establish a unified picture of how electronically adaptive ligands reshape transition metal bonding. This work advances our understanding of metal–ligand interactions and provides a framework for rational design in catalysis and materials chemistry.

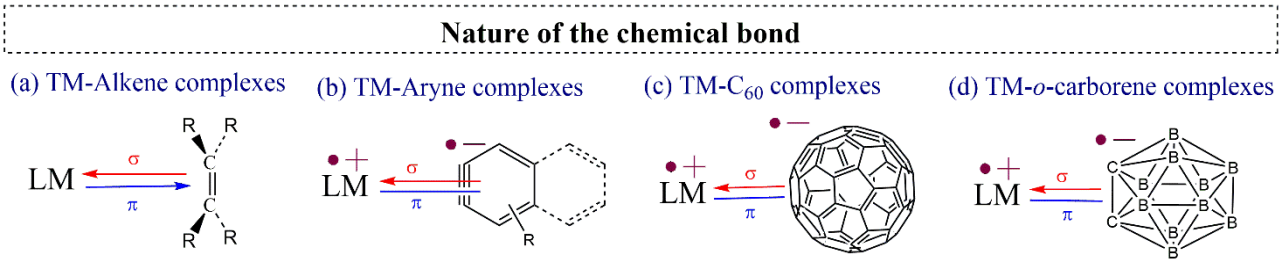


Figure 1: The different bonding scenarios in different transition metal-ligand complexes.

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Theoretical Chemistry Symposium
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Computational Insights into the Heavy Atom Influence on Intramolecular ISC in Azabenzanthracene Derivatives

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Azabenzanthracene (AzBA) derivatives have recently gained significant attention owing to their promising applications in organic electronics, photodynamic therapy, and fluorescence imaging[1,2]. Despite their potential, the photophysical properties of these derivatives, particularly their intersystem crossing (ISC) dynamics, remain poorly understood. In this work, we investigate the photophysical properties of AzBA derivatives, with a particular focus on the effect of heavy-atom substitution. Using time-dependent density functional theory (TDDFT) calculations performed with the Q-Chem 5.4 package[3,4], we demonstrate that bromination significantly enhances spin–orbit coupling (SOC), leading to ultrafast ISC and high triplet yields.

Notably, 12-bromo-1-azabenzanthracene (12-Br-1-AzBA) exhibits an ultrafast ISC rate of $10^{12} s^{-1}$, calculated according to Marcus theory[5]. This high rate results from the synergistic effects of the heavy-atom effect, favourable orbital angular momentum transitions from the $^1\pi\pi^*$ to the $^3n\pi^*$ state, and an optimal singlet–triplet energy gap. Additionally, the lateral overlap between the pyridinic nitrogen n-orbital and bromine's in-plane p-orbital extends conjugation, further amplifying spin–orbit coupling. Interestingly, the position of bromine substitution has minimal impact on the fluorescence rate constant, which remains approximately $10^7 s^{-1}$. These insights establish design principles for tuning ISC dynamics in azabenzanthracenes, offering a molecular platform for developing advanced materials with tailored photophysical properties.

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Computational Study on Gold(I) Acetylide Complex Formation and Tandem A^3 Coupling/Cyclization for Aminoindolizine Synthesis

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Gold(I) acetylide complexes efficiently carried out one-pot tandem A^3-coupling/cyclization reactions of alkyne, amine, and pyridine-2-carboxaldehyde, yielding pharmaceutically important nitrogen-based bicyclic amino indolizines.[1] In this study, we computationally explored the interrelated synthetic pathways among various gold(I) derivatives, namely, aryl thiolato, acetylido, and chloro analogs, from a mechanistic standpoint, as such a comparative investigation has not been previously conducted. Furthermore, the density functional theory (DFT) studies performed on a representative gold(I) acetylide complex reveal that the synthesis of aminoindolizine proceeds through a two−step gold(I)−catalyzed tandem A^3−coupling and cyclization mechanism.[2] DFT computations further revealed that Au•••H−C and van der Waals interactions play an important role in facilitating A^3-coupling and subsequent cyclization. The observed kinetic barriers in these transformations are modulated by the cooperative participation of both aliphatic and aromatic Au•••H−C interactions, underscoring their significant influence in gold catalysis. The DFT study demonstrates that the 1,2−hydrogen transfer is the rate-limiting step for the entire tandem A^3−coupling followed by cyclization mechanism.

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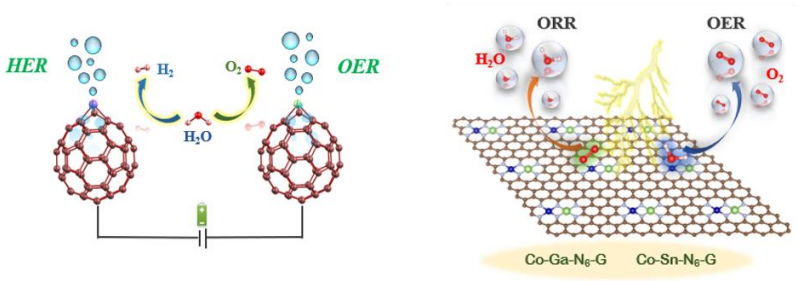
Computational Modelling of metal doped carbon nanostructures for electrochemical water splitting and metal air battery applications

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The growing demand for sustainable energy has intensified the search for efficient and cost-effective electrocatalysts for water splitting and metal-air batteries, particularly due to the adverse impacts of fossil fuels. Single- and bi-atom catalysts have emerged as highly promising candidates for key electrochemical reactions such as the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR).

In this poster, we present the catalytic applications of transition metal (TM)-doped carbon-based nanostructures, specifically graphene and fullerene for renewable energy applications. Using density functional theory (DFT), we investigate TM doped (Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt) fullerene as electrocatalyst for water splitting.[1] The results indicate that sixth-row TMs, particularly Ir and Pt, exhibit outstanding HER activity, while fifth-row metals such as Ru and Pd show superior performance in OER. In a separate study, the bifunctional electrocatalytic performance for metal air battery is examined for TM (Fe, Co, Ni) co-doped nitrogen-doped graphene systems (TM-N_6-G) by introducing p-block metals (PM = Al, Ga, In, Sn, Bi) into an N_4 cavity, resulting in TM-PM-N_6-G structures.[2] Systematic DFT calculations reveal that Co-Ga-N_6-G and Co-Sn-N_6-G configurations exhibit remarkable bifunctional catalytic performance for OER and ORR, with several others unifuncional catalysts. The Co centers act as the active sites for OER/ORR, while the PM atoms play a crucial role in enhancing the catalytic activity of the transition-metal centers.

The enhanced catalytic activity is attributed to optimal interactions with reaction intermediates, as supported by scaling relations and volcano plots. The influence of the electronic structure is elucidated through band-center and COHP analyses, charge distribution on the metal centers, and contour maps. Furthermore, correlation functions are analyzed to propose a new descriptor for designing efficient bifunctional catalysts. Thermal stability of the most promising catalysts is assessed using AIMD simulations.



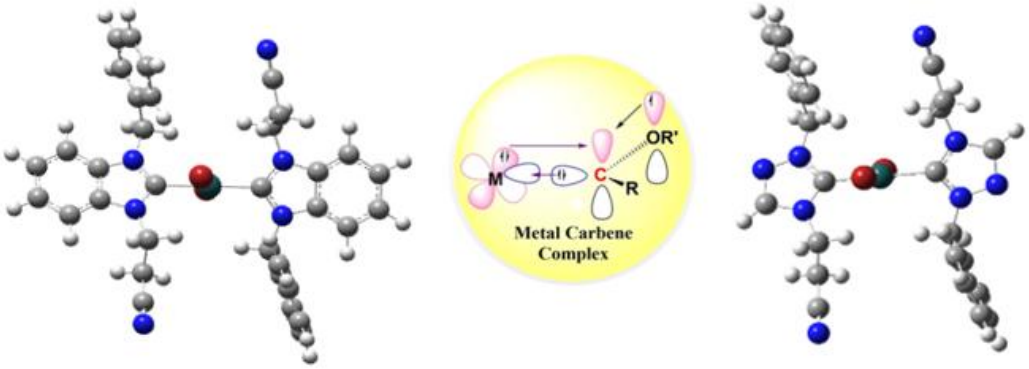
(a) (b)

Figure 1: (a) Transition-metal-doped fullerene exhibits efficient electrocatalytic water splitting activity. (b) p-block and transition metal-doped N-graphene demonstrate bifunctional electrocatalytic activity for OER and ORR.

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Electronic Origin of Carbene Carbon on Hydrogen Evolution Reaction (HER): Experiment and Theoretical Studies

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The electronic origin of ligand effects is crucial for advancing molecular electrocatalysts for the hydrogen evolution reaction (HER). In this study, we investigated the role of the carbene carbon in palladium (II) bis-N-heterocyclic carbene (NHC) complexes derived from triazole and benzimidazole scaffolds. The carbene carbon center serves as a strong σ-donor/π-acceptor,[1,2] modulating electron density at the Pd center and thereby tuning hydrogen adsorption–desorption energetics. Electrochemical investigations demonstrated that ligand architecture governs HER activity, with triazole-based complexes exhibiting superior performance compared to benzimidazole analogues. To probe the molecular origin of these trends, density functional theory (DFT) calculations were carried out, including geometry optimizations and frequency analyses to confirm structural stability. Electronic structure analysis from density of states (DOS) revealed strong contributions from carbene carbon orbitals to Pd d-states, indicating effective electronic coupling. Crystal orbital Hamilton population (COHP) and crystal orbital bond index (COBI) analyses further established that triazole-derived carbenes form stronger Pd–C bonding interactions, enhancing Pd–H stabilization during catalysis. This combined experimental–theoretical study establishes the carbene carbon as the key electronic origin of catalytic activity in Pd–NHC complexes and provides electronic-level design principles for tailoring ligand frameworks in next-generation HER electrocatalysts.

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TD-DFT and Molecular Dynamics calculations to Determine the selectivity of G-quadruplexes by a molecular rotor with an ESIPT emission

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A basic photochemical mechanism known as excited-state intramolecular proton transfer (ESIPT) has been studied for many years. Due to its potential use is it has been receiving a lot of interest in the realm of metal-organic optical materials because of its extensive photophysical capabilities[1]. This change occurs at a very high speed, frequently in the sub-100 fs range. Nowadays, a wide range of theoretical techniques at various levels are accessible to assist and direct practical studies, even if its experimental characterization might be quite difficult. We conducted a comprehensive theoretical investigation of molecular excited state trends and ESIPT techniques for the new, highly miscible sophoflavescenol[2] molecule in this study. The ESIPT reaction usually involves a four-stage photophysical process called photoinduced tautomerism. Typically, ESIPT fluorophores exist in the ground state (S0) as enol. Photoexcitation may be used to excite the fluorophores to the excited state (S1). In this viewpoint, we provide an overview of the most recent developments in quantum chemistry techniques together with tools from molecular and quantum dynamics that have been effectively used in ESIPT process investigations. We emphasize a careful evaluation of their distinct characteristics.

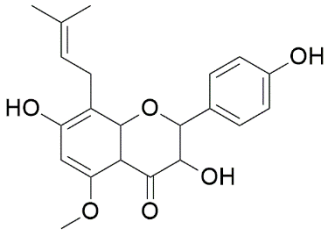


Figure 1: Sophoflavescenol

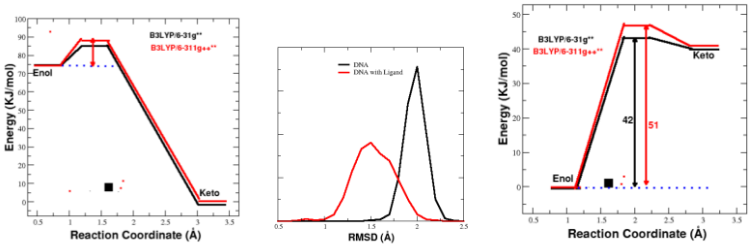


Figure 2: TD-DFT calculations and MD Simulation (RMSD) analysis

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GaN Epitaxial Growth along m-Plane (1-100)

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Epitaxial growth of Gallium Nitride (GaN) crystals on non-polar *m*-plane is crucial for manufacturing LED devices with higher efficiency. GaN crystals with a lower density of defects and dislocations can be produced by growing films on a vicinal surface, which induces 'step-flow' growth[1]. We have constructed lattice-based kinetic Monte Carlo (kMC) simulations of *m*-GaN growth and used it to growth on planar and vicinal m-plane surfaces.

Quantum mechanical calculations have shown that, adsorbed N atoms on m-plane GaN surfaces form strong N-N bonds with the surface N atoms. This leads to weakening of the surface N bonds and subsequent desorption in the form of N_2 molecules[2]. In our kMC simulations, we have incorporated this desorption process in addition to the typical processes of deposition of Ga and N atoms and thermal hopping of the surface atoms. We observed the evolution of various surface morphologies with variation in growth parameters. Our results qualitatively match those observed in molecular beam epitaxy experiments, where it is seen that excess nitrogen flux leads to smooth growth involving step flow along [000-1] direction. Additionally, our results follow the observed behavior with variation in miscut angle and miscut direction. Based on our observations, we have located the optimum growth conditions for step flow growth under moderate temperature and deposition flux.

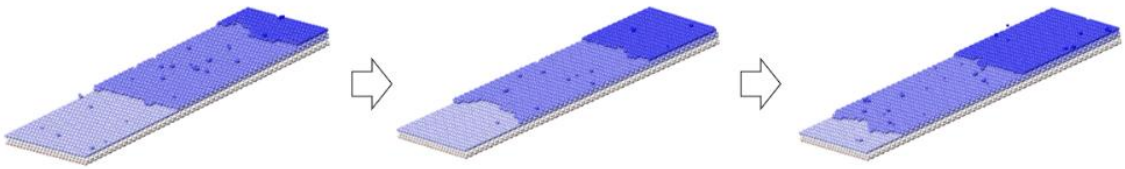


Figure 1 Step-flow in *m*-GaN growth: Deep blue color denotes larger surface height

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Linear Response and Quantum Work Statistics

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Guarnieri et al. [1] recently showed that the full generating function of dissipated work can be derived within linear response theory. They demonstrated that the entire work distribution is encoded in a single quantity—the standard relaxation function of the autocorrelation. This result allows phenomenological models to study non-equilibrium fluctuations in complex quantum systems. We extend their framework by linking it more directly to Kubo's formalism. In doing so, we move beyond autocorrelations and show how the response of any observable can be systematically related to generalized correlation functions [2]. We apply this to cross-correlations, highlighting their role in the thermodynamic uncertainty relation through the Fano factor and dissipated work. This also leads us to a refined notion of relaxation time that better captures non-equilibrium dynamics. Finally, our formulation unifies linear response with quantum work statistics. It recovers well-known fluctuation theorems such as Jarzynski's equality, Crooks' theorem, and the Evans–Searles relation, thereby providing a more general framework for non-equilibrium quantum thermodynamics.

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Viscosity Dependence of Deep Eutectic Solvents on Cation and Anion Identity

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Mixing of two or more individual components at a definite mole fraction forms Deep Eutectic Solvents (DESs), which remain in liquid state at around room temperature(1,3). In acetamide+thiocyanate based DESs simply changing from Na^+ to K^+ viscosity changes from 1805 cp to 339 cp. Nearly an order of magnitude difference in viscosity due to difference in cation identity profoundly impact their physicochemical properties(4). In contrast, we do not observe such drastic change in viscosity in acetamide + nitrate based DESs. In this work we report the molecular level understanding behind this ion-specific viscosity behaviours for these DESs by using Molecular Dynamics Simulations. Interaction energy between cation and anion indicates that in acetamide+nitrate based DESs viscosity varies due to cation-anion interaction, whereas a complex interplay of multiple ion-ion and solute-ion interactions dictated the strong viscosity dependence for acetamide+thiocyanate based DESs. Further analysis by computing radial distribution function, Voronoi polyhedra,diffusion coefficient, non-gaussian parameter provides a molecular level insight into how subtle changes in ion composition can affect the physicochemical properties of deep eutectic solvents.

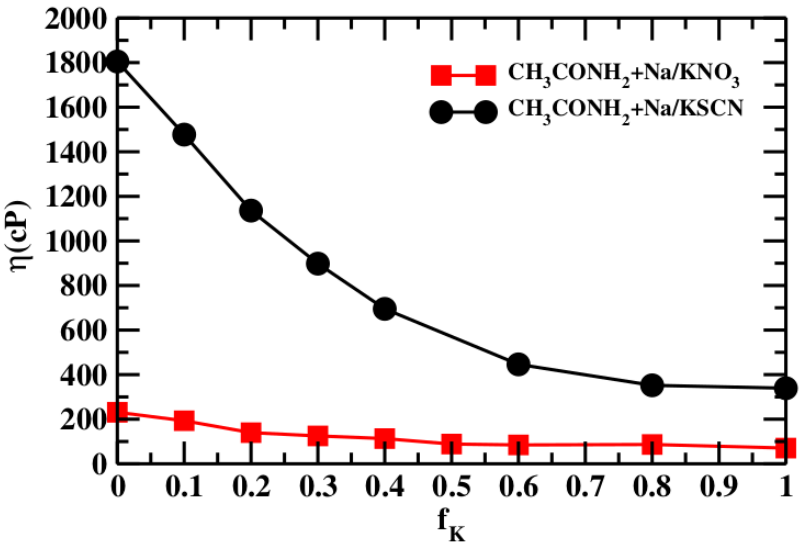
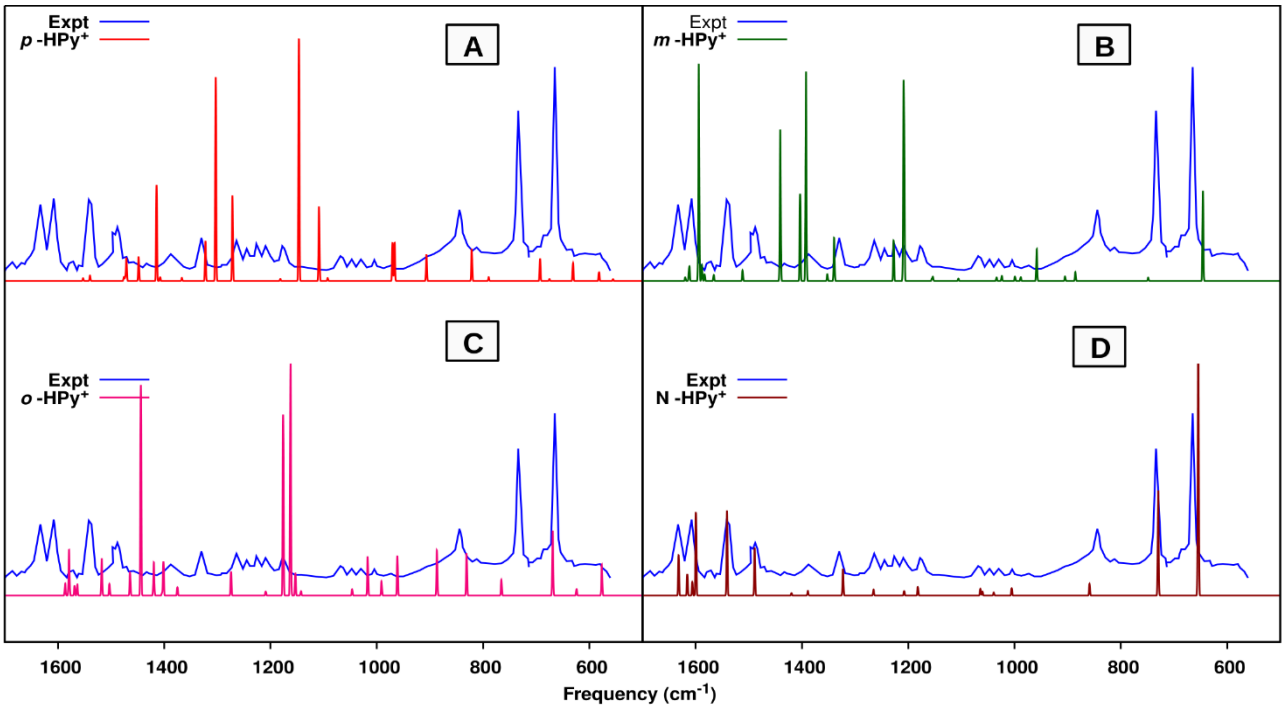


Fig. Viscosity as a function of mole fraction of potassium(f_K)

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Ab initio investigation of the IR spectrum of neutral pyridine and protonated pyridine: A vibrational coupled cluster study

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The IR transitions of protonated pyridine cation and neutral pyridine are studied using the Vibrational Coupled Cluster Method (VCCM). The in-situ experimental spectrum is likely due to the mixture of different conformers and undissociated pyridine[1,2]. The results indicate that the spectrum is mainly due to transitions for the lowest energy conformers and the undissociated molecule. The analysis shows that the effect of the positions of protonation and cationic charge plays a significant role in the transition frequencies and intensities. We analysed the dipole moment functions of different conformers of this interstellar system to understand the variation of the signature IR peaks in the torsion region.

Figure 1: Comparison of IR spectral values obtained from VCCM calculations with the experimental data for protonated pyridine conformers in the range between 600-1600 cm^{-1}

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Tracing the Origin of Non-Aromatic UV-vis Absorption and Emission in Proteins: Study of Lysine and Glutamate Dimers.

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Over the past decade, a growing body of experimental evidence has highlighted the emergence of unusual (nonaromatic) fluorescence in biomolecular systems. The signals intensify in aggregated states, with prominent examples including amyloid structures[1,2], condensates[3] and monomeric proteins enriched in charged amino acids[4]. At present the precise molecular mechanism and the nature of the chromophore(s) remains elusive, several hypotheses have been proposed which are being under intense study[5]. In this poster, we identify special structural motifs within charged amino acid clusters (lysine-glutamate dimers) which can produce unusual UV-vis absorption features in proteins termed Protein Charge Transfer Spectra (ProCharTS)[4]. Specifically, we deploy TDDFT spectral analysis and dimensionality reduction techniques to understand various geometrical features in the lysine-glutamate dimers influencing absorption wavelengths. Further, we develop a generalised Smoluchowski equation approach[6] to model excited state relaxation and time-dependent fluorescence in charged amino acid dimers. We will present results obtained on one-dimensional harmonic free-energy surfaces for the ground and excited states. We will discuss further applications to ProCharTS as well as red-edge excitation spectroscopy (REES).

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Transient Occupancy and Pore Dynamics: IP6 behavior in HIV-1 T=4 Capsids

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HIV-1's genome is enclosed in a conical capsid made of capsid proteins (CA), which protects it and regulates key replication events.[1] The HIV-1 CA must maintain a balance between stability and flexibility in order to support key stages of the viral life cycle. Inositol hexakisphosphate (IP6), a negatively charged cellular metabolite, contributes to this balance by interacting with the electropositive pores of CA oligomers, particularly through coordination with residue Arg18.[2] HIV-1 capsid is not restricted to a single strict morphology. Factors like chemical cross-linking, salt concentration, or mutations can shift capsid morphology.[3,4] R18A and R18L mutations without IP6 mainly produce spherical particles, similar to T=4 icosahedrons, in high-salt conditions, showing a direct connection between R18 and capsid shape.[5,6] We performed extensive all-atom molecular dynamics simulations on T=4 icosahedral capsids in the presence and absence of IP6, as well as the R18L mutation, to gain insights into how local molecular interactions shape global capsid behavior. We find that IP6 binding to pentameric pores is energetically favorable, but the β-hairpin and R18 ring create kinetic barriers that restrict spontaneous IP6 movement, in contrast to the more accessible hexameric pores. Importantly, the local binding events, including the R18L mutation, cause minimal alterations to global capsid dynamics and ion transport. These results suggest that overall capsid geometry plays a dominant role in determining large-scale mechanical behavior, and that IP6 functions as a dynamic stabilizer rather than a strict architectural requirement.

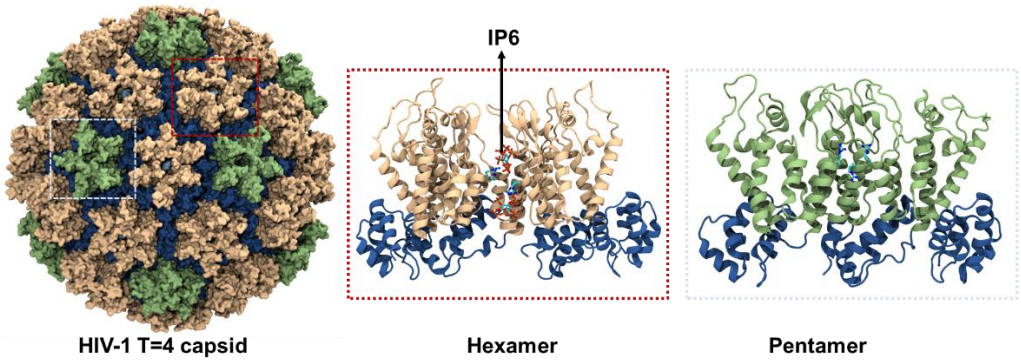


Figure 1 HIV-1 T=4 model and the representative hexamer and pentamer structures.

References:

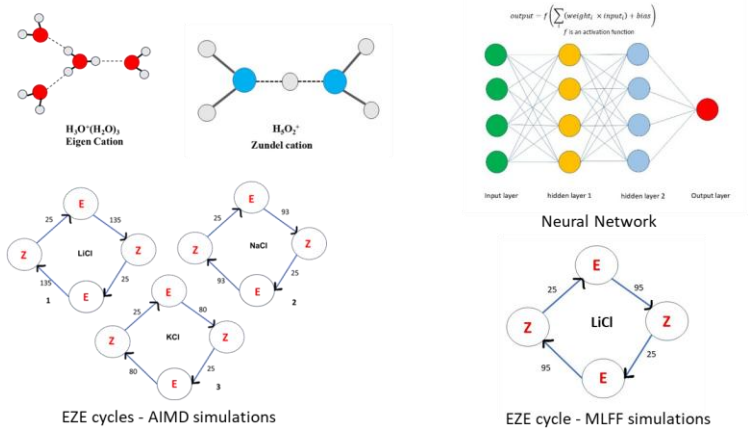
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Computational Insights into the Impact of Alkali Metal Salts on the Hydrated Proton Structure and Eigen-Zundel Interconversion

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Various chemical and biological reactions have proton transfer as one of the ubiquitous components in them.[1] The solvation structure of the proton plays a critical role in determining the mechanism and kinetics of proton transfer. In water, it is known to adopt two forms, Eigen cation, $H_9O_4^+$ and Zundel cation, $H_5O_2^+$.[2,3] The proton transfer mechanism primarily follows an Eigen-Zundel-Eigen (EZE) mechanism, where a distorted Eigen cation is the most stable structure, and the Zundel cation is an intermediate complex.[4] Molecular dynamics (MD) simulations probe the structure and transfer mechanisms of hydrated hydronium ions. Accurate proton transfer modeling requires detailed structures and long trajectories, but *ab inito* MD (AIMD) is costly and classical MD lacks accuracy. Therefore, machine learning force fields (MLFF), especially neural network potentials (NNP), have been employed to address these limitations. NNPs provide a solution by reproducing first-principles energies and forces using machine learning algorithms. In this study, we trained NNPs for pure water, acidic water, and salt-containing acidic water systems, combining AIMD and MLFF-based MD to examine how alkali metal salts influence hydrated proton structure, lifetime, and transfer mechanisms. We found that the Eigen cation is the most stable hydrated form, persisting longer than the Zundel cation. Moreover, while Eigen cation lifetimes varied with different cations, the Zundel cation lifetime remained unchanged.



The numbers on the arrows denote the time in fs for which Eigen(E) and Zundel(Z) cations are stable.

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Design of high transformation temperature shape memory alloys with low hysteresis using first-principles study

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The quest for high-temperature shape memory alloys (SMAs) with low hysteresis has driven extensive research over the past several decades due to their potential in industrial and biomedical applications.[1,2] Among various alloying strategies, equiatomic NiTi remains the base system of choice, with Hf and Cu identified as particularly promising dopants: Hf enhances transformation temperatures, whereas Cu reduces hysteresis.[3,4] However, systematically identifying optimal compositions remains challenging, as experimental exploration demands substantial resources and often fails to fully capture the microscopic mechanisms—such as compositional effects, lattice dynamics, and entropy contributions—that govern transformation behavior.[5]

In this work, we investigated the compositional dependence of transformation properties in NiTi-based SMAs by introducing controlled amounts of Hf (11.11–36.11 at.%) and Cu (2.78–22.22 at.%) concentrations into $Ni_{18}Ti_{18}$ through the substitution of Ti and Ni atoms, respectively. Using the special quasi-random structure (SQS) algorithm, we constructed atomistically randomized models of the B2, B19, B19′, and B33 phases for $Ni_{18-x}Ti_{18-y}Hf_yCu_x$ ($x = y = 0$, and $1 \leq x \leq 8$; $4 \leq y \leq 13$) compositions. We systematically evaluated their phase energetics and lattice vibrational spectra. Our analysis established clear correlations between dopant concentration and key observables.

These results provide critical insight into the role of alloying on phase stability and transformation behavior, and thereby offer valuable guidance for the rational design of next-generation high-temperature SMAs. The detailed findings will be presented and discussed.

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Theoretical Chemistry Symposium
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Demystifying the Reaction Mechanism of Asymmetric Photocatalytic de Mayo Reaction

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In recent years, photoredox catalysis has emerged as a sustainable and versatile platform in radical chemistry, allowing a wide range of organic reactions to proceed under mild conditions. These processes hinge on exothermic single-electron transfer (SET) steps, which in turn depend on the redox potential of the photocatalyst(s). However, the limited redox range of excited-state photosensitizers often restricts their scope. To overcome this, König and co-workers proposed sensitization-initiated electron transfer (SenIET) mechanism, where polycyclic aromatic hydrocarbons (PAHs) act as cosensitizers to enable energy accumulation through Dexter energy transfer (EnT).[1] In our work, we have computationally investigated the photocatalytic cycle of the asymmetric photocatalytic de Mayo reaction which happens to give no net yield without the involvement of a PAH cosensitizer moiety.[2] We have particularly focussed on the Dexter EnT and SET processes to decipher the role of the cosensitizer and the catalytic process as a whole. We have used a combination of Density functional theory (DFT) and classical Marcus theory as tools to estimate free energy barriers of SETs and EnT steps.[3] Sun X. *et al*. had suggested that the cosensitizer coordinated substrate is the species responsible for EnT.[2] On the contrary, our results demonstrate that the cosensitizer is directly involved in EnT and is the standalone character in this process. The computed barriers are in agreeable range accounting for the facileness of this reaction under mild conditions. These findings reveal key factors governing SenIET and can potentially provide a blueprint for designing next-generation photocatalysts and cosensitizers for plethora of photoredox reactions.

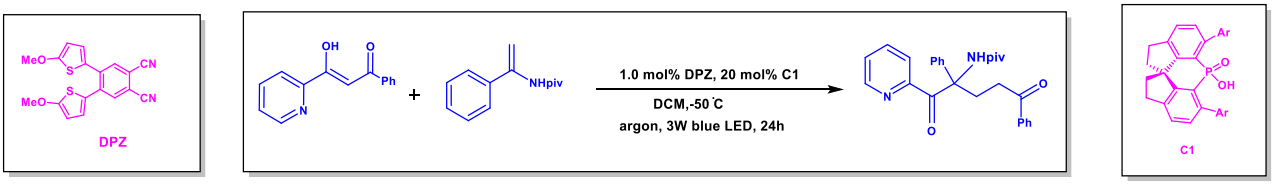


Figure1: Asymmetric photocatalytic de Mayo reaction catalysed by dicyanopyrazine (DPZ) and a PAH cosensitizer

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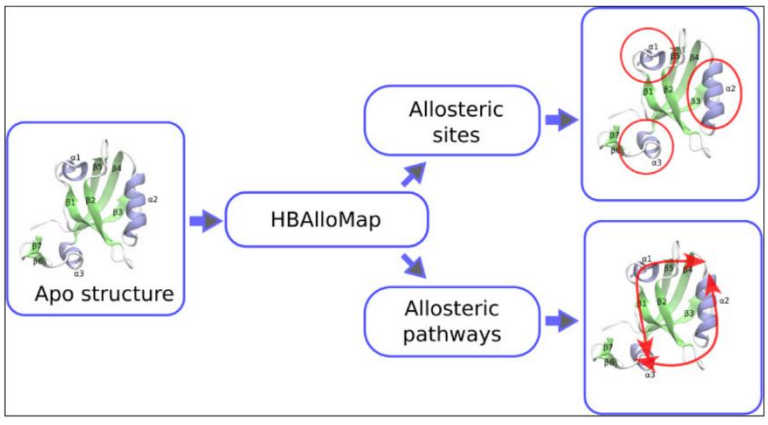
Hydrogen Bond Allosteric Map (HBAlloMap): Mapping Allostery from Apo-State Hydrogen Bond Fluctuation Correlation

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Allosteric regulation enables long-range functional coupling in biomolecules, yet the quantitative identification of allosteric sites and signal transduction pathways remains a major theoretical and computational challenge. Here, we present Hydrogen Bond Allosteric Map (HBAlloMap), a correlation-based framework that decodes allosteric networks by analyzing statistical covariances among hydrogen bond fluctuations obtained from equilibrium molecular dynamics (MD) simulations of the apo state.

Our central hypothesis is that intra-protein hydrogen bonds not only stabilize local structure but also act as dynamical conduits for allosteric signal propagation. We construct time-resolved Hydrogen bond binary matrix and compute the covariance matrix of hydrogen bond occupancy fluctuations, followed by eigenmode decomposition to extract principal dynamic coupling patterns. By ranking residues according to their projection along dominant eigenvectors, HBAlloMap identifies putative allosteric hotspots and reconstructs signal transduction pathways.

Application to different proteins show that this approach quantitatively recovers known allosteric hotspots and signal transduction pathways. These findings support the view that the apo-state ensemble harbors latent information about functional connectivity, encoded in its fluctuation spectrum. HBAlloMap thus offers a thermodynamics-grounded route to decoding allosteric architecture from equilibrium dynamics.



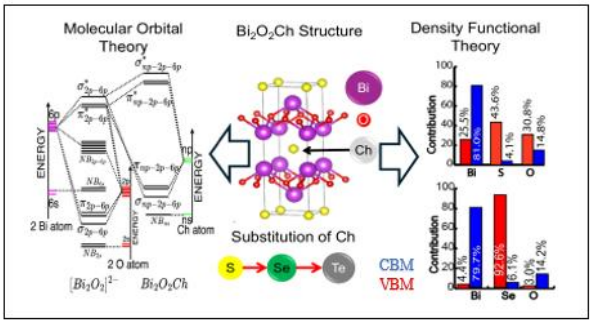
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Determining the Principles for Designing Electronic Band Structures of Complex Materials with Desired Properties

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Electronic band structure determines how atomic-level interactions influence the electrical and optical behavior of material. If we understand the priniples for tuning the band structures, we can rationally design materials with desired electronic, optical, and topological properties. However achieving such control remains challeng because band structure emerge from complex inter-orbital interactions and atomic hybridization effects. Even small changes in structure or composition can modify orbital overlap, crystal-field splitting and spin orbit effects, leading to significant changes in electronic band structure. Density functional theory gives us accurate band structure but it have lack of information about the mechanism of orbital interation to form a electronic band structure. In this work we combine analytical molecular orbital theory[2] (MOT) with numerical DFT and tight-binding model[3] (TBM) to determine the physics that controls the electronic band structure formation with the orbital interaction view. We used layered Bi_2O_2Ch (Ch = S, Se, Te) as an example because of its crystal structure and the tunable chemistry. This combined method gives better understanding of how orbitals and atoms work to form the band structure, something that DFT cannot explain on its own. In this study MO analysis clears the narrowing using chalcogen p hybridization and stronger Bi–O antibonding. DFT calculations confirm indirect band gap decreases from Bi_2O_2S to Bi_2O_2Te, with O-2p and Ch np states forming the VBM and Bi 6p forming the CBM. In addition to explain the orbital coupling and SOC effects, a Slater–Koster[4] Tight-Binding model replicates DFT trends. This combined method provides both computational accuracy and physical insight by bridging the gap between first-principles calculations and atomic-level orbital theory. It demonstrates that band-gap evolution can be systematically controlled by tuning orbital interactions. This approach greatly lowers the cost and time of conventional trial-and-error methods by integrating MOT, DFT, and TB modeling to enable data-driven inverse design of materials with desired electronic and optical properties.



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Analysis of High-Dimensional Free Energy Landscapes Using Neural Network

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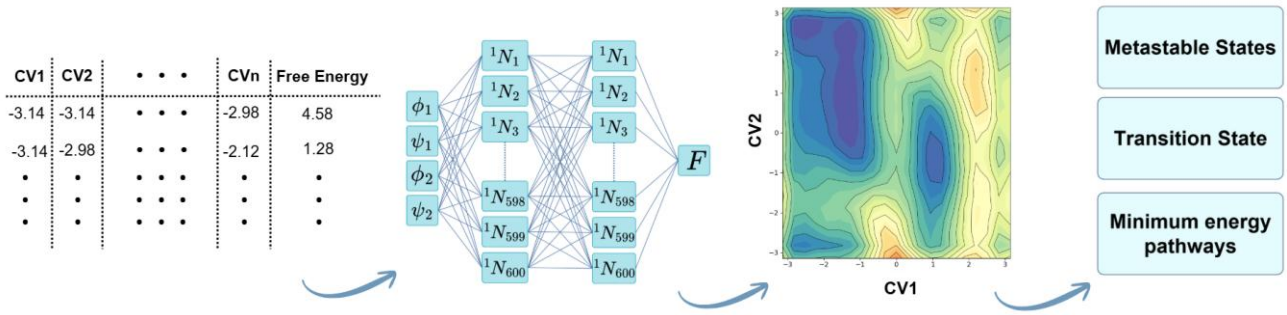
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Free Energy Surfaces (FES) as a function of reaction coordinates provide critical insights into chemical and biological reactions by revealing all possible molecular states. In molecular dynamics and enhanced sampling[1] studies, these surfaces are typically visualized as grid data along relevant coordinates, known as collective variables (CVs). However, for complex reactions involving multiple metastable states, a large number of CVs becomes necessary, leading to high-dimensional free energy surfaces that are noisy and challenging to analyze.

To overcome this and accurately identify reaction pathways, we employ artificial neural networks (ANNs) to derive a compact, analytical representation of the high-dimensional grid data.[2] Here, we propose a novel approach for the efficient identification of metastable states and minimum energy pathways using the ANN-generated analytical FES. In this work, we demonstrate results for alanine tripeptide, which can be further scaled to larger biomolecules, enabling automated exploration of high-dimensional free energy landscapes and facilitating the discovery of novel molecular mechanisms.



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Role of B Concentration on the Activity of Graphene-Supported Single-Atom Catalysts for CO_2 Reduction to CH_4

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Single-atom catalysts (SACs) have emerged as a promising candidate for electro-catalytic CO_2 reduction reaction (CO_2RR), offering remarkable atomic utilization and exceptional selectivity. The catalytic activity of SACs is believed to be largely influenced by the choice of support. Among various 2D supports, graphene has emerged as a popular support for transition metal (TM) SACs, off-late. Recently, boron (B)-doped graphene (B-Gr) has shown potential as a catalyst for conversion of CO_2 into HCOOH, and B-Gr supported Cu cluster has been promising in the formation of C_2 product in CO_2RR . However, TM SAs embedded B-Gr as potential catalysts for CO_2RR still remain relatively under-explored. Furthermore, the effect of varying B-concentration in graphene on the activity, stability and selectivity of the TM SACs is yet to be understood thoroughly. Addressing this gap, our present work systematically assess the influence of varied B concentration (B_x-Gr, x = 1, 2, 3) on the catalytic properties of 4*d* and 5*d* TM SAs, (Mo, Ru, Os and Pt), anchored on B-doped graphene, employing density functional theory (DFT). Our DFT results also show that all the TM@B_x-Gr (B_x-Gr, x = 1, 2, 3) catalysts efficiently activate CO_2, a step pivotal for efficient CO_2RR. Our bader charge analysis revealed that a substantial charge transfer from the TM SAs to CO_2, facilitates the activation in CO_2. Additionally, our selectivity analysis suggests that except Mo@B_1-Gr, Ru@B_3-Gr, and Pt@B_3-Gr, all other TM SACs are selective towards CO_2RR over the competetitve hydrogen evolution reaction (HER). Finally, from the Gibbs free energy calculations it is evident that Os- and Pt-doped B_x-Gr (x = 1, 2) preferentially reduce CO_2 to CH_4, while the rest of the catalysts predominantly yield HCOOH. Notably, Os@B_1-Gr exhibits an impressive limiting potential of -0.49 V for CH_4 formation. Through DFT-based calculations and analysis, our study showcases and explains the intricate effect of varying dopant concentration on the activity of the TM SACs towards CO_2RR.

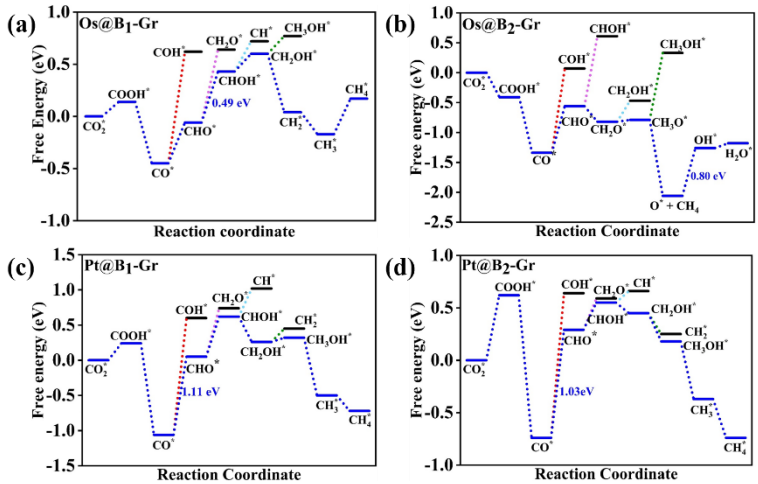


Figure 1. Reaction free energy profile for the preferred pathway on **(a)** Os@B_1-Gr, **(b)** Os@B_2-Gr, **(c)** Pt@B_1-Gr and **(d)** Pt@B_2-Gr.

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A Monte Carlo Simulated Annealing-Based Computational Protocol for Modeling High-Entropy Alloy Structures for Electrocatalytic Studies

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High-entropy alloys (HEAs), composed of five or more principal elements in near-equimolar ratios, represent a novel class of materials that form stable solid-solution structures with high configurational entropy.[1] These materials have recently attracted interest for electrocatalytic applications due to their chemical complexity, tunable surface properties, and compositional flexibility.[2,3] While there are computational studies that explored the electrocatalytic activity of HEAs, comprehensive insights into their structure-property-activity relationships across the vast compositional space remain limited.[4] Statistical mechanics-based methods, such as Monte Carlo simulations, are therefore essential to identify thermodynamically stable atomic configurations of HEAs. Conventionally, special quasirandom structures (SQS) are employed to generate HEA configurations purely based on configurational entropy.[5] In this work, we present a robust computational protocol for modeling the CoCrFeMnNi HEA, a 3*d* transition metal system of high interest due to the individual catalytic activity of its constituents for processes such as electrochemical nitrogen reduction reaction (NRR), yet largely unexplored experimentally in electrocatalysis. Our approach generates representative structures that closely approximate experimentally relevant configurations by combining SQS-based initial structure generation, Monte Carlo simulated annealing-based screening with a modified embedded-atom method (MEAM) force field, and validation using density functional theory (DFT) calculations. The resulting configurations, with appropriate supercell sizes, can be directly employed for surface slab generation, adsorption studies, and subsequent catalytic investigations.

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Heat as a Pattern Architect: Thermal Modulation of Spatiotemporal Instabilities in Reaction–Diffusion Systems

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Self-organization in reaction–diffusion (RD) systems gives rise to a rich variety of spatiotemporal patterns, ranging from stationary Turing structures to complex oscillatory dynamics. In this study, we investigate the chlorine dioxide–iodine–malonic acid (CDIMA) reaction–diffusion system, focusing on the role of temperature as a critical control parameter in the emergence and stability of self-organized patterns. While the CDIMA system is well-known for producing Turing patterns under nonequilibrium conditions[1,2], the influence of thermal variations on its pattern-forming as well as homogeneous regimes remains largely unexplored. Through a combination of analytical modeling and numerical simulations, we examine how temperature affects reaction kinetics via the Arrhenius-type equation[3], thereby modulating the onset of instabilities. Our results reveal that increasing temperature shifts the boundaries between homogeneous, stationary, and oscillatory regimes. In particular, we identify scaling behaviors indicating that even small thermal perturbations can reorganize the entire spatiotemporal pattern landscape.

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Theoretical Chemistry Symposium
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Role of Conformational Flexibility of an Inhibitor on its Dynamic Interactions with Ribonuclease A

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The inhibition of Ribonuclease A (RNase A) has gained significant attention due to its therapeutic potential, particularly in angiogenesis and the digestion of dietary RNAs, where controlling RNA turnover is crucial. We report in this work computer simulation studies on the molecular mechanism of inhibition of RNase A by a selected molecule, i.e., 5'-phospho-2'-deoxyuridine-3'-pyrophosphate adenosine-3'-phosphate (pdUppA-3'-p) or PUA, which has already been experimentally synthesized (K_i = 27 nM) and is known to target different aspects of the active site of the enzyme and overall structural dynamics[1]. However, the presence of a flexible pyrophosphate moiety in the inhibitor raises questions about its inhibition efficiency, as this may be strongly dependent on conformational preferences (Figure 1). Integrating classical molecular dynamics with steered molecular dynamics (SMD)[2] and umbrella sampling (US)[3], the stability and conformational dynamics of RNase A in complex with the inhibitor across its accessible conformations have been evaluated, and contributions originating from rare fluctuations have been identified at and around the active site. Our findings suggest that a critical aspect of the inhibitory mechanism is governed by conformation-specific interactions that modulate both the bound and unbound states of RNase A.

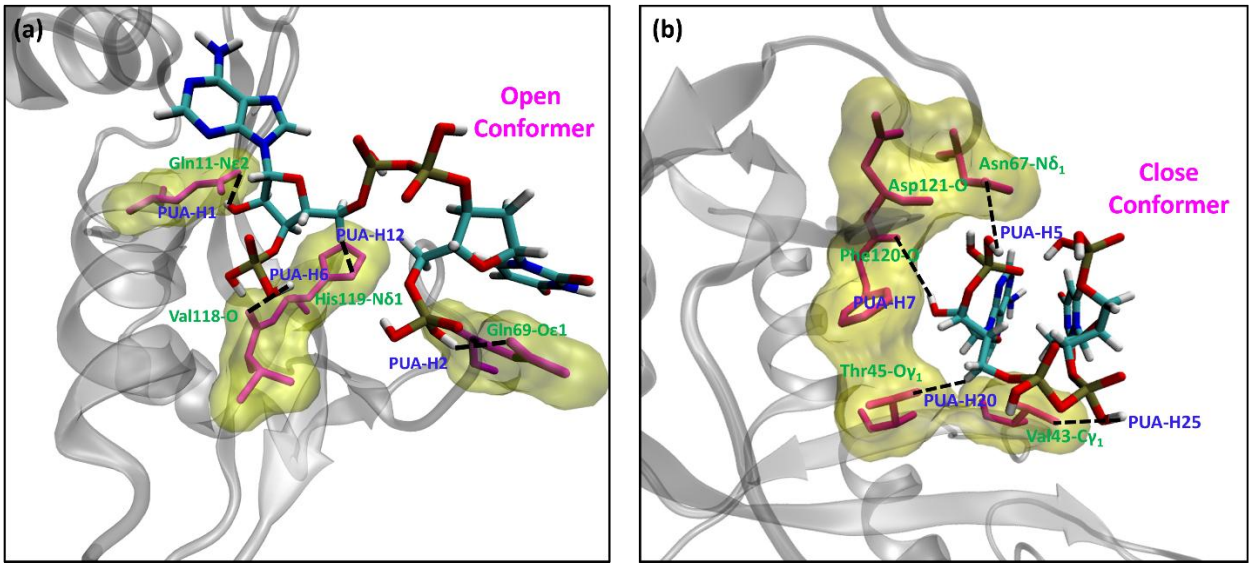


Figure 1 Schematic illustration of the interactions between the inhibitor (PUA) and the active site residues in the open (a) and closed (b) conformational states of the inhibitor.

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First-Principles Screening of 3d Transition-Metal Trimers on h-BN for Electrocatalytic NO to NH_3 Reduction

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The electrochemical reduction of NO to NH_3 is drawing significant research interest as an alternative to the Haber-Bosch process and for reducing NO emissions. Recent studies show that metal cluster-modified catalysts provide more active sites for this reaction. In this study, we systematically investigated the activation of NO on trimeric clusters of transition metal atoms anchored on hexagonal boron nitride (h-BN) (Fig. 1a). Ten first-row transition metals (TM_3 = Sc to Zn) were selected for evaluation. The performance of TM_3-BN was assessed based on charge transfer during NO adsorption and dissociation, as well as metal–NO charge transfer (Fig. 1b). In addition, orbital hybridization between the nitrogen p orbitals and the d orbitals of the transition metals was analyzed via partial density of states (PDOS) (Fig. 1c), and bond activation was confirmed through integrated crystal orbital Hamilton population (ICOHP) analysis (Fig. 1d). TM_3-BN catalysts were evaluated based on two criteria: (i) NO adsorption and (ii) HER inhibition. More generally, catalysts for reduction reactions must satisfy three requirements: (i) stability, (ii) activity, and (iii) selectivity.Conclusively, Cu_3 and Mn_3 clusters emerged as the most effective catalysts for the NO reduction reaction (NORR), fulfilling these criteria. They demonstrated high stability with suppressed HER activity, enhanced NO adsorption and activation, and superior NH_3 selectivity, exhibiting the lowest limiting potentials of U_L = –0.29 eV and U_L = –0.46 eV, respectively.

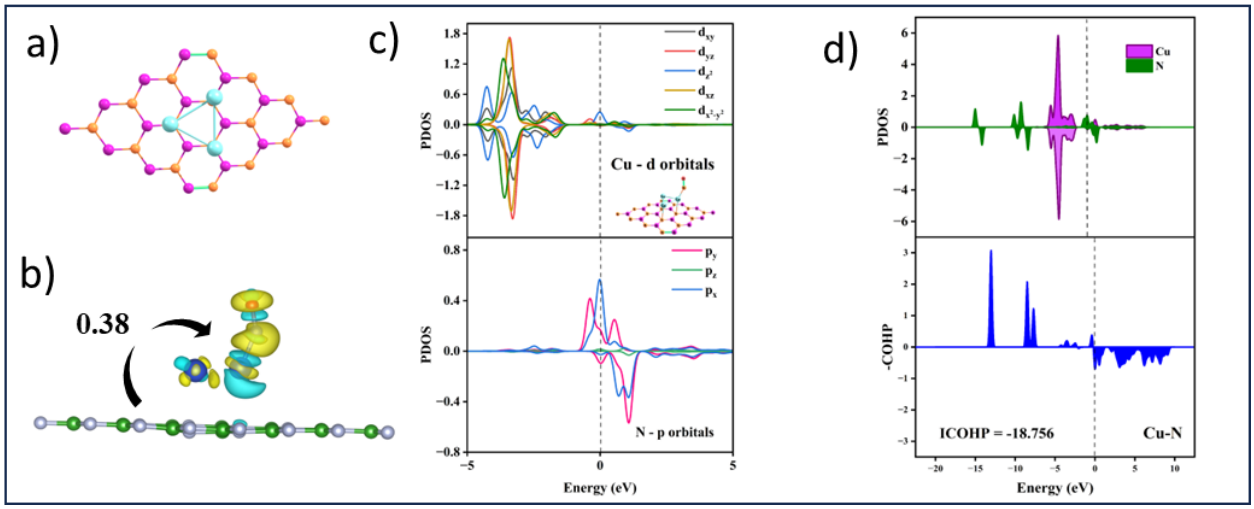


Figure 1 a) Optimized structure of Cu_3-h-BN **b)** Charge transfer between h-BN and Cu_3 **c)** Partial Density of States of Cu_3 and N atoms **d)** Crystal orbital Hamiltonian population between Cu and N

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Off-Diagonal Thermodynamic Contributions as Predictors of Selectivity in Nonheme Iron-Catalyzed Halogenation

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Iron-catalyzed selective halogenation of alkanes represents a compelling biomimetic strategy to emulate nonheme halogenases and probe the fundamental mechanisms of C–H bond functionalization. Previous studies by Comba and co-workers (2016) revealed striking ligand-dependent trends in chlorination selectivity for iron(II) complexes supported by tetradentate ligands: bispidine (L1) achieved 100% chlorination, TQA (L2) ~70%, TPA (L3) ~40%, and PTACN (L4) displayed negligible selectivity. These results underscore the decisive influence of ligand architecture on the rebound step and the competition between halogenation and hydroxylation pathways.[1]

Despite previous observations, the mechanistic origin of selectivity in these systems remains unclear. In this work, we employ a comprehensive set of theoretical methods to gain insight into this issue. Our approach includes standard Eyring transition state theory, analysis of the reactive mode composition during the H-atom abstraction (HAA) step and its influence on post-HAA trajectories (e.g., Cl vs. OH rebound), evaluation of the impact of three-component thermodynamics on the HAA barrier and subsequent selectivity, as well as molecular dynamics simulations. Together, these methods not only rationalize the observed trend in chlorination efficiency (L1 > L2 > L3 > L4), but also provide actionable guidance for the design of next-generation, highly selective nonheme iron halogenation catalysts.

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Singlet fission in dimer to aggregate : a tensor network based approach

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Singlet fission (SF) provides a route to utilise the wasted energy of the solar spectrum by creating two triplet excitons from one singlet exciton. Two general classes of molecules that show SF are acenes and polyenes (carotenoids). Owing to the complicated excited state manifold and different electron correlation, the understanding of SF process in carotenoids, unlike acenes, remains obscure. We provide a combined electronic and vibronic picture for a polyene model system that unravel the mechanism of SF in this class. We show that the dark multiconfigurational A_g states and charge transfer (CT) states play important roles in dictating the mechanism. The process is further propagated by bond length alternating (BLA) high frequency vibrational modes.[1,2]

We also provide a spin-resolved tight-binding excitonic model for SF that can be parameterized based on ab initio calculations on monomers and dimers of molecules, and is highly suitable for the study of aggregates using tensor network methods such as the density matrix renormalization group.[3] This tensor network coarse-grained model is demonstrated specifically on the pentacene crystal, where we evaluate the spectra and density of states. We show the natural emergence of bands of states in some cases, and characterize them. Through an analysis of entanglement entropy of the eigenstates, we gain crucial insight into the extent of their multireference character.

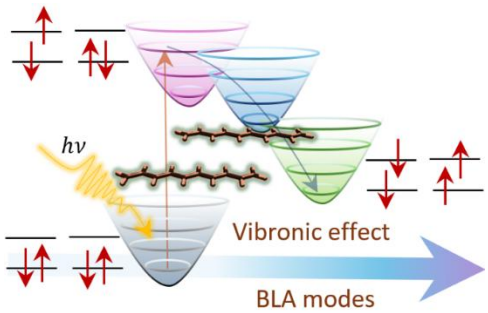


Figure 1 Schematic representation of the SF process in Carotenoids

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Collective Effects in Cavity-Coupled Jahn-Teller Active Molecules

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We study the polaritonic states and dynamics of multiple Jahn–Teller (JT) active molecules coupled to the modes of a Fabry–Perot cavity[1]. We find that collective effects dramatically alter the interplay of electronic, vibrational and cavity angular momenta, giving rise to markedly different polaritonic spectra and dynamics even when going from one to two JT molecules. Starting from the ground vibronic state, we find that JT molecules[2,3] collectively coupled to a common cavity can access high-angular-momentum vibronic states in the presence of a single cavity photon, in sharp contrast to the single molecule case where the range of accessible angular momentum values are bounded. We show that such collective photonic–vibronic couplings lead to an efficient cavity-mediated vibronic angu- lar momentum transfer between molecules. The observable consequences are broadening of the cavity–molecular polariton spectra, and a strong coherent response of the cavity- photon polarization dynamics to an external broadband polarized light pulse. Our results shed light on how new angular momentum transfer mechanisms are enabled by collective coupling and present consequences for the chemical and physical applications of molecular polaritonics.

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Machine Learning-based improved descriptor for ^{13}C NMR chemical shift prediction of small organic molecules.

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In the atoms-in-molecules (AIM) machine learning (ML) approach, the *descriptor* or *representation* is a mathematical mapping of the atomic environment to predict the atomic properties of a molecule[1]. In this study, we investigate the fundamental backbone that underlies the discrete and continuous representations for predicting the ^{13}C-NMR chemical shift in the QM9NMR dataset[2]. The conversion of discrete to continuous function descriptors is applied for popular physics-based descriptors, the Coulomb matrix (CM)[3] and bags-of-bonds (BoB)[4]. To make the descriptor more informative, *n* nearest-neighbor atomic information is also embedded in the parent descriptor. Using the radial basis function and the local versions of the CM and BoB descriptors, we construct the following four descriptors: aCM(*n*), aBoB(*n*), aCM-RBF(*n*), and aBoB-RBF(*n*). In the kernel ridge regression (KRR) ML architecture, the descriptor shows an improvement with increasing neighbor *n*, and becomes constant with further increase. The aBoB-RBF(4) is found to be the best, with a mean absolute error of 1.69 ppm, which improves upon previously reported ML-KRR models[5]. The KRR-aBoB-RBF(4) model is further tested for many validation molecular datasets and is found to give accurate results, even for larger molecules, showing the ability of the aBoB-RBF(4) descriptor to be transferable to larger molecules. Furthermore, when the nearest-neighbor inclusion is applied to aSLATM[6], a three-body descriptor, the improvement in accuracy due to neighbor inclusion is minimal, indicating that the nearest neighbor can capture many-body effects. We also found the importance of the conformational effect of the molecular geometry in training the ML model, which is aimed at future work.

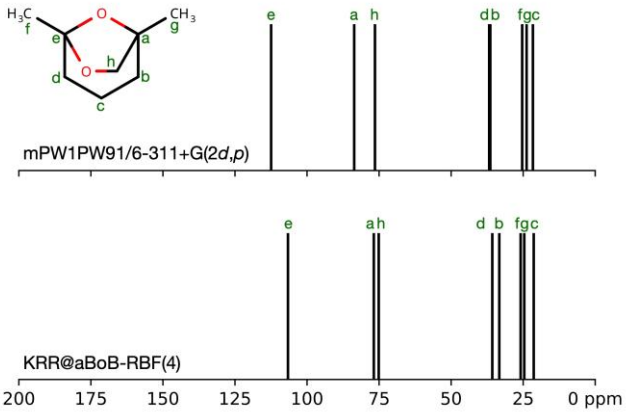


Figure 1: DFT versus ML-based prediction of 13C-NMR chemical shifts.

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Exploring Spin Transport Characteristics of Mixed-Valence {V^{IV}-V^{III}} Magnetic Dimer: Probing the Interplay of Magnetic-Exchange and Double-Exchange Effects

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This study delves into the exploration of coherent transport properties of single-molecule junction (SMJ – Figure 1) devices featuring the molecule [$(Me_3tacn)_2V_2(CN)_4(\mu\text{-}C_4N_4)$] (**1**).[1,2] Employing a combination of DFT, ab initio CASSCF/NEVPT2 and NEGF calculations, we explored the spin state energetics, magnetic properties, and quantum transport characteristics of these complexes, aiming to uncover their potential applications in molecular spintronics devices.[3-6] The complex **1**, upon one-electron reduction (**1**$_{red}$), exhibited Robin-Day class III mixed-valence magnetic dimer characteristics. The neutral state displayed strong antiferromagnetic coupling, which switched to ferromagnetic upon reduction. DFT calculations revealed an antiferromagnetic exchange interaction of -97 cm^{-1} between the V^{IV} centres, consistent with the experimental reported value of -112 cm^{-1}. The TD-DFT calculations confirmed strong intervalence charge transfer in reduced state, making S = 3/2 the ground state with the double-exchange parameter, B>>J. Quantum transport studies showed greater conductance in the high-spin state (S_T = 1) compared to the broken symmetry state (S_T = 0) in 1, attributed to the presence of *β*-empty states in the conduction band near Fermi energy. The 1_{red} exhibited an enhanced spin transport characteristics due to complete electron delocalization between the V centres. Notably, our Quantum transport studies unveiled a large spin-filtering efficiency of around 95.5% for complex **1** and 74.6% for **1**$_{red}$.

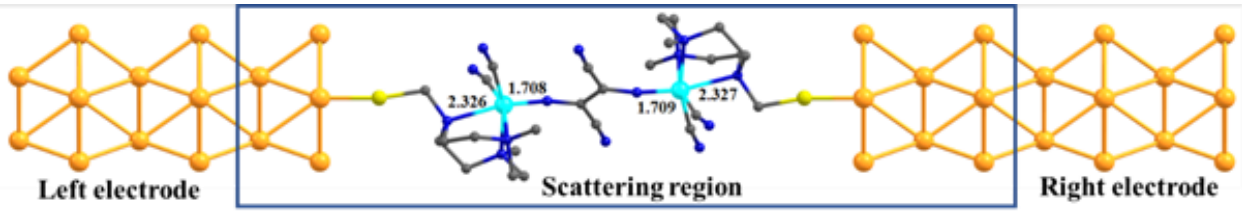


Figure 1. SMJ device to compute the quantum transport properties through the complex **1**$_{red}$.

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Theoretical Chemistry Symposium
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Atmospheric Oxidation of Pyruvonitrile and Formyl Cyanide: Mechanistic Insights and Kinetic Evaluation with OH Radicals and Cl Atoms

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The atmospheric degradation of (RCOCN, where R = CH_3 and H) plays a significant role in understanding the fate of nitrogen-containing oxygenated volatile organic compounds (OVOCs).[1] In this study, we investigate the gas-phase reactions of RCOCN with hydroxyl (OH) radicals and chlorine (Cl) atoms utilising Density functional theory (DFT) calculations and kinetic modelling. Potential energy surfaces (PES) were constructed at the CCSD(T)/CBS//BHandHLYP/cc-pVTZ level to explore the detailed reaction pathways. Only one hydrogen abstraction site (RCOCN, where R = CH_3 and H) is feasible in this case. Rate constants were computed over a relevant atmospheric temperature range (200-400 K) using canonical variational transition state theory (CVT) with small-curvature tunnelling (SCT) corrections.[2] This study contributes to the broader understanding of nitrogenous OVOCs chemistry in the troposphere by providing a comprehensive mechanistic and kinetic understanding of (RCOCN, where R = CH_3 and H) oxidation, as well as discussing atmospheric implications such as lifetimes and degradation products.

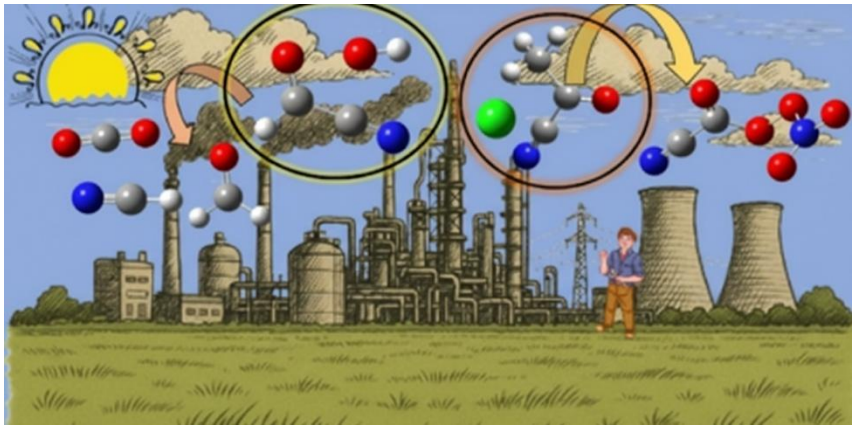


Figure 1. Degradation mechanism of RCOCN (where R = CH_3 and H).

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Molecular Interaction in Mixtures of Pyrrolidinium-based Ionic Liquids and Water : Computer Simulation Studies

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In this study, we perform comprehensive molecular dynamics simulations to investigate the structural and transport properties of pyrrolidinium-based ionic liquids in presence of varied water content. Using the re-optimized CL&P force field and SPC/E water model, simulations were carried out at 298~K and 1~bar to assess the effects of cosolvent (H_2O) concentration on key physicochemical properties. The results reveal non-monotonic density trend, sharp decline in viscosity, and significant enhancement in diffusion coefficients and ionic conductivity with increasing water mole fraction. The dielectric constant of the mixtures rises steeply, indicating dominant dipolar effects of water at higher water ration. Hydrogen bond contact analysis further confirms the disruption of ion–ion interactions and the formation of strong ion–water associations. These findings demonstrate the pivotal role of water in modulating the microscopic environment and dynamic behavior of ionic liquid (IL) systems and provide critical insights for designing tunable, eco-friendly IL–cosolvent mixtures for green solvent applications.

Reference:

1. Molecular Dynamics Simulation Studies to Investigate the Interactions between Pyrrolidinium-based Ionic Liquids and Water.
Sushree Sangita Moharana[#], Kavita Thakran[#], Suthar Shravankumar Tejaram, Praval Pratap Singh, Chandraniv Dey, and Sudip Chakraborty* (Submitted)

#These authors contributed equally to this work.

Theoretical Chemistry Symposium
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Solubility predictions and role of solvents using machine learning algorithms

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Abstract

Solubility prediction remains a longstanding challenge in drug development due to the complex interplay of molecular structure, solvent environment, and temperature. Traditional physics-based models, while informative, often struggle with generalization and scalability. Here, we implemented a machine learning approach to predict solubility based on molecular fragments and experimental conditions for a wide range of solute–solvent systems. Out of multiple regression models tested, Random Forest proved to be the best performer, achieving high accuracy and strong generalization to novel data. Rigorously designed data cleaning processes, descriptor selection, and hyperparameter optimization were all critical parts of the Random Forest model workflow. Learning curve and data split analyses further revealed several training set characteristics and feature distribution critical for capturing order and disorder across solubility spaces. The findings illustrate that machine learning tools provide accurate, scalable, and interpretable solubility prediction-underpinned with applications in initial drug candidate evaluation and formulation development.

Model Name	R2		MAE		RMSE	
	train	test	train	test	train	test
Linear Regression	0.47	0.47	0.67	0.67	0.89	0.89
Random Forest	1.00	0.98	0.04	0.09	0.08	0.17
Gradient Boosting	0.63	0.62	0.57	0.58	0.74	0.75
SVM	0.98	0.94	0.09	0.15	0.19	0.30

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Electronic Structure of the Metal-Nitrenoid Intermediate Governs Intramolecular C–H Amination Mechanism

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The formation of metal-nitrenoid (M–NR) intermediates is a critical step for transition metal-catalyzed C–H amination reactions. While a majority of intermolecular C–H amination reactions with azide nitrene precursors require extrusion of N_2 molecules for the formation of the M–NR species, the intramolecular amination reactions involving anthranil substrates undergo ring-opening pathways for the nitrenoid formation. Here, we report an unprecedented correlation between the nature of ring-opening and the subsequent mechanism of C–H amination. A Cp*Co(III)-catalysed intramolecular C–H amination of anthranil was investigated to uncover how the electronic nature of the nitrenoid governs the overall reaction mechanism. The mechanistic and electronic structure investigation outlines the evolution of the bonding scenario across the [C–N–Co] core (Figure 1) as the determining factor for the subsequent amination pathway. Overall, these investigations revealed that anthranil derivatives undergo “unconventional” ring opening facilitated by electron donation from the aryl ring at the C7 position to form a unique cobalt-nitrenoid species, which follows an electrocyclization pathway to achieve the intramolecular C−H amination.

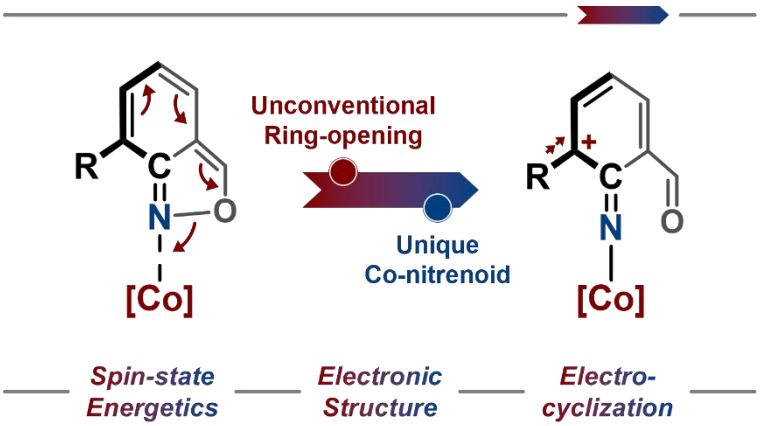


Figure 1. Formation of Co-nitrenoid via unconventional ring-opening governs the C–H amination by the electrocyclization pathway.

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An Evolutionary Algorithm for The Designing New Singlet Fission Molecules

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Genetic algorithm is an optimization technique inspired by natural evolution.[1] In this approach, candidates “evolve” over generations through selection, mutation, and crossover to optimize a desired property. In this work, we present a genetic algorithm for the automated discovery of new organic molecules with potential singlet fission activity.[1] Molecules are encoded using SELFIES and modified through a variety of mutation operations, enabling the algorithm to explore chemical space in a guided yet diverse manner.[1] Each generation is evaluated for chemical viability. DFT/TDDFT methods are used to optimize molecular structures and calculate excitation energies. This approach provides a systematic and efficient strategy for discovering new molecular structures with desired properties, paving the way for the accelerated design of advanced organic materials.

References:

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Structural motifs of Semiconducting 2D Boron based on polyhedral B_{12}

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The boron analog of graphene is being extensively explored for a diverse range of technological applications. All theoretically predicted atomically thin borophenes are metallic and remain experimentally elusive in their free-standing form, presumably due to their high reactivity, similar to that of silicene. Interestingly, the experimentally characterized semiconducting nanosheets are reported to be B_{12}-based, as determined by microscopic imaging, although the detailed structures remain unknown. Since the B_{12} unit is essentially 3D, some of its exopolyhedral bonds must be absent and may form exo-π bonding[2] (as in benzyne). Our DFT inquiry shows that the polyhedral B_{12}- the building block for all boron allotropes –promises to be a superior structural motif for boron's 2D avatar as well. Exploration of various topologies reveals structures that show a definite band gap when the dianionic requirement of B_{12} unit is satisfied through multicentered exohedral π or σ bonding– between[3] or within[2] the B_{12} units– respectively. Though the pronounced sp dissonance of boron[4] makes its π-type lateral overlap less effective, the curved B_{12} surface facilitates its formation, which passivates the frontier.Their dynamic stability is confirmed by phonon spectra. The most stable among them (Figure 1) is 14.29 kcal/mol higher in energy than α-rhombohedral boron, yet isoenergetic to the most stable borophene sheet χ_3.

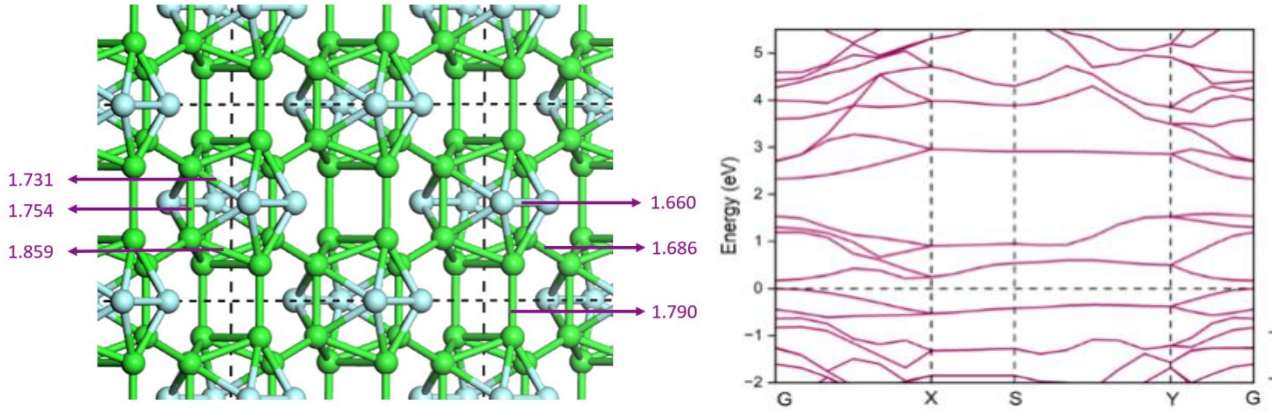


Figure 1. (a) Structure of the unit cell (p2mg) where bare boron (without exohedral bond) is colored distinctly. (b) Its direct band gap at Gamma (CGA/PBE @ 575eV plane wave cutoff).

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A Multireference Framework for Calculating X-ray Absorption Near-Edge Spectra (XANES) of Transition-Metal Complexes

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X-ray absorption spectroscopy (XAS) provides critical insights into the electronic structure of transition-metal complexes, with broad applications in chemistry and biology.[1] In this work, we focus on the K-edge spectra of 3d transition-metal complexes, benchmarking different computational approaches across common oxidation states and ligand environments. Time-dependent density functional theory (TDDFT) and restricted open-shell configurational interaction singles (ROCIS) perform reliably for states dominated by single excitations but fail to capture features arising from strong multiexcitonic character. In contrast, modified ROCIS (ROCIS*) and multiconfigurational methods such as restricted active space self-consistent field (RASSCF), restricted active space second-order perturbation theory (RASPT2), and multiconfiguration pair-density functional theory (MC-PDFT) provide robust and accurate descriptions of the pre-edge region.[1,1] Our results demonstrate that orbital optimization within the MCSCF framework is crucial, and that including the metal 1s and 3d orbitals in the active space is sufficient to capture all the peaks in this region. Additionally, relativistic effects and basis set choice strongly affect the empirical energy shift required for spectral alignment. These findings highlight the importance of multiconfigurational methods and active-space design for reliable simulation of K-edge XAS in transition-metal complexes.

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Cyclo-Stationary Distributions of mRNA and Protein Counts for Random Cell Division Times

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There is a long history of using experimental and computational approaches to study noise in single-cell levels of mRNA and proteins. The noise originates from myriad factors: intrinsic processes of gene expression, partitioning errors during division, and extrinsic effects, such as random cell-cycle times. Although theoretical methods are well developed to analytically understand the statistics of copy numbers for fixed or Erlang distributed cell cycle times, the general problem of random division times is still open. For any random (but uncorrelated) division time distribution, we present a method to address this challenging problem and obtain exact series representations of the copy number distributions in the cyclo-stationary state. We provide explicit cell age-specific and age-averaged results, and analyze the relative contribution to noise from intrinsic and extrinsic sources. Our analytical approach will aid the analysis of single-cell expression data and help in disentangling the impact of variability in division time s.

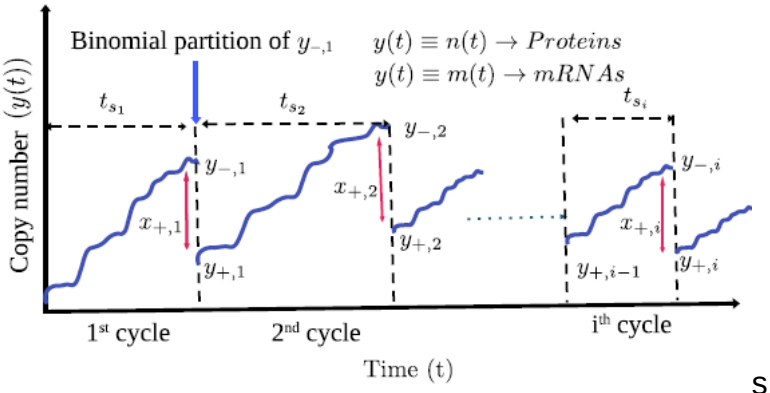


Figure 1 Schematic diagram of time evolving copy number, of either mRNA [m(t)] or proteins [n(t)] in successive generations, interrupted by cell divisions when the number $y_{-,i}$ binomially divides to $x_{+,i}$ and $y_{+,i}$ in the two daughter cells. The durations t_{si} of the cell cycles are random and drawn from a probability distribution $g(t_s)$. After several generations i>>1, the copy numbers attained a cyclo-stationary distribution.

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Cellular uptake of microgels by membrane wrapping

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The interaction of nano- and microparticles with lipid-bilayer membranes plays a key role in the process of cellular engulfment.[1] The physico-chemical parameters that control engulfment are size, shape, elasticity of the particle, and bending rigidity, tension of the membrane, and particle-membrane adhesion strength.[2] Stimuli-responsive polymeric microgels are particularly versatile because their elasticity can be tuned in a wide range by changing the density of crosslinkers. Using continuum models of spring networks for the microgels, and triangulated surfaces with Helfrich's curvature elasticity for the membrane, we study microgels wrapping at lipid-bilayers,[3] where microgels are attached to the membranes via ligand-receptor bonds. Hertz theory is employed to characterize the microgel's Young's modulus and Poisson's ratio. The interplay of microgel and membrane deformations is controlled by the competition between microgel elasticity and membrane bending rigidity. Our numerical simulations predict an increased stability of partial-wrapped states for microgels at lower Young's moduli. There is a discontinuous transition from oblate to nearly spherical microgels with increasing wrapping fractions, irrespective of membrane tension. Volume and surface area of partial-wrapped microgels are significantly reduced compared with those of free microgels.[3] Understanding microgel wrapping will facilitate the design of tunable and responsive polymeric gels for biomedical applications, e.g., targetged drug delivery vectors.

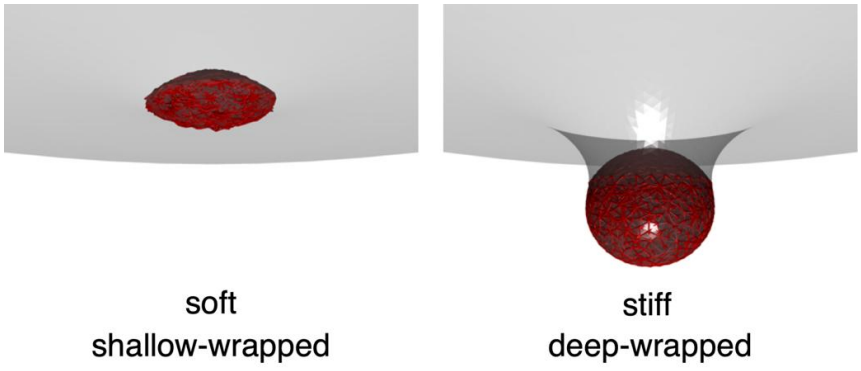


Figure 1 Stable wrapping states for soft and stiff microgels with same adhesion fraction

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Theoretical Chemistry Symposium
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Exploring How Metal–Oxo Identity (Fe, Co, Mn) Governs C–H Activation in Ethylene-Forming Enzymes

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Abstract: The selective activation of aliphatic C–H bonds remains a central challenge in catalysis due to their inertness and high bond dissociation energies.[1-3] Among biological systems, nonheme Fe(IV)=O species have emerged as key oxidants capable of promoting such transformations, notably in ethylene-forming enzymes (EFEs), where they facilitate L-arginine oxidation via efficient C–H activation.[3] In this study, we investigated the effect of metal substitution in EFEs by replacing iron with cobalt and manganese to understand how metal identity influences catalytic reactivity. Through extensive molecular dynamics (MD) simulations, we probed the structural flexibility and stability of the Fe, Co, and Mn variants. Local Electric field (LEF) analyses were conducted to quantify protein-generated local electrostatic effects during the trajectory and in key intermediates. Hybrid QM/MM calculations were employed to map out the energy landscapes and spin-state preferences across metal-substituted systems. Furthermore, multireference CASSCF calculations revealed significant differences in spin-state mixing and wavefunction character, providing insights into the electronic factors that govern C–H bond activation efficiency. Our findings establish a strong correlation between electric field directionality, spin-state energetics, and reactivity, offering a comprehensive understanding of how metal substitution modulates catalytic behavior in EFE-like systems

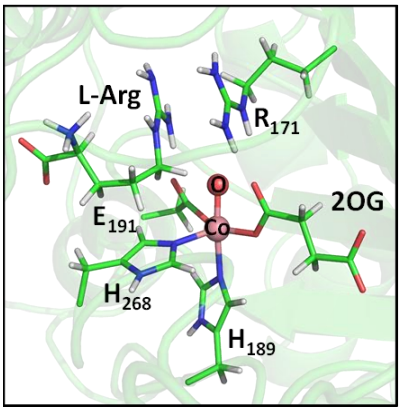


Figure 1: Representative MD-derived structure of the Co^{IV}=O species in EFE, highlighting Glu_{191}, His_{268}, His_{189}, 2-α-ketoglutarate, L-arginine (substrate), and Arg_{171}, with Arg_{171} forming a hydrogen bond to the oxo group of Co^{IV}=O.

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Insights into xylan-cellulose interactions to improve biomass deconstruction for sustainable biofuel production

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The structural integrity of plant cell walls presents a major challenge in the efficient conversion of biomass to biofuels[1]. A major factor contributing to this recalcitrance is the interaction between cellulose and hemicellulose, particularly xylan, the most abundant hemicellulose in nature. Xylan often has acetyl (Ac) group substitutions along its backbone, which are known to impact its structural conformation and interaction with cellulose microfibrils[2,3,4]. The present work investigated the effect of xylan acetylation on its interaction with cellulose surfaces using unrestrained molecular dynamics (MD) simulations. Our findings reveal that all acetylated xylan exhibit a ≈10-40% higher 2-fold screw population on the (100) hydrophobic surface compared to the (110) hydrophilic cellulose surface, suggesting enhanced interactions due to higher number of hydrophobic contacts of xylan with cellulose. Interestingly, xylan with non-periodic acetylation showed reduced propensity to form 2-fold screw conformations, despite maintaining comparable number of hydrogen bonding and overall contacts with cellulose surfaces. This highlights the critical role of both substitution pattern and surface topology in mediating xylan-cellulose interactions. Highly acetylated xylans (>50%) desorb from cellulose , while low acetylated forms exhibited surface-dependent binding behavior. The findings further imply that a specific and unique set of xylan-cellulose interactions stabilize the 2-fold screw conformation of xylan. These findings contribute to a deeper understanding of plant cell wall architecture and offer a potential basis for designing efficient biomass deconstruction strategies in biofuel production.

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Theoretical Chemistry Symposium
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Thermodynamic Insights into Biomimetic Quantum Batteries

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Abstract

We propose a five level theoretical model of a quantum battery inspired by bacterial light-harvesting complexes. In our design, collective quantum optical subradiant and superradiant states take on distinct roles for energy storage, retention, and use. The charging, leakage, and storage dynamics are quantified using expectation values obtained from a quantum master equation that tracks the time evolution of the interacting states. Transition rates are derived from an effective non-Hermitian Hamiltonian that reflects the battery's geometry. We evaluate complete thermodynamic performance, including ergotropy, work extraction, flux, and power. Each function reaches maximum efficiency at specific ring sizes optimized for its role. Strong coupling between the ring and central system boosts energy storage capacity but lowers achievable power output. By systematically varying key parameters such as dipole count, inter-dipole coupling strengths (J_d), detuning (Δ), charging reservoir temperature (T_c) and cavity temperature (T_w), the model identifies optimal geometric configurations that maximize operational figures of merit. This establishes a direct connection between microscopic dipolar interactions and open-system thermodynamics, with collective photonic effects governing the balance between rapid charging through superradiant channels and long-lived storage in subradiant states. This work provides insights into designing quantum batteries by learning from biological systems that have evolved to capture and manage energy.

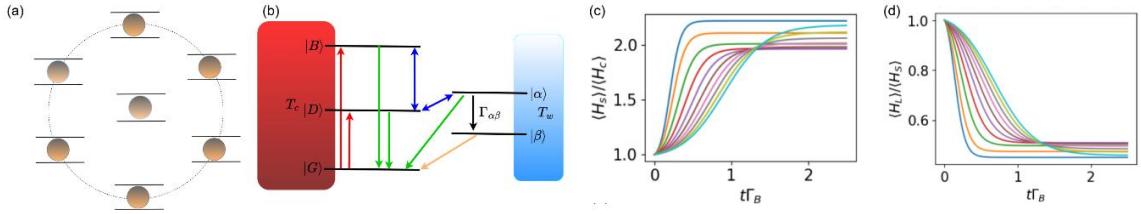


Figure 1(a) - (d) A symmetric ring of two-level systems coupled to a detuned central system forms bright and dark states, where {|B⟩,|D⟩,|G⟩} couple to a charging reservoir (T_c) and {|α⟩,|β⟩} to a cavity (T_w)

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Theoretical Modelling of Molecular Crystals to Doped Nanocrystals: From Tunable Triplet Emission to Radiative Recombination

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Core substitution to a class of n-type arylene diimide semiconductors, known as pyromellitic diimides (PmDIs), not only induces a wide spectrum of fluorescent colors but, enables a wide-range of phosphorescence spanning across visible spectra. In this context, we have worked on various core-substituted PmDIs, which were synthesized and photophysical studies were carried out by Prof. George's group. We have demonstrated how core substitution enables the precise modulation of triplet-state emission, spanning over 190 nm across the visible spectrum and in some cases, shows simultaneous presence of intense phosphorescence as well as TADF[1].

Extending this theme of emission control through molecular/atomic-level design, we explored Zn-doping in $CsPbI_3$ perovskite nanocrystals (PNCs). $CsPbI_3$ PNCs exhibit an absorption band-edge around 670 nm, enabling broader utilization of the solar spectrum compared to other halide perovskites. Unlike Mn^{2+}/Ni^{2+}, Zn^{2+} possess filled *d*-orbitals that lie deep in the valence band, potentially suppressing non-radiative losses while promoting radiative decay. In fact, Prof. Mandal's group reported that Zn-doped $CsPbI_3$ PNC showed gigantic molar extinction coefficient, $\varepsilon \approx 2 \times 10^8$ M^{-1} cm^{-1} and PLQY ≈ 0.98, making it super-absorber and super-bright among quantum dot-PNC family.[2] Using *ab-initio* calculations, we attributed this exceptional PLQY to charge carrier localization at the Zn (dopant) site, extending carrier lifetime and suppressing non-radiative losses, thereby facilitating efficient light emission.[3]

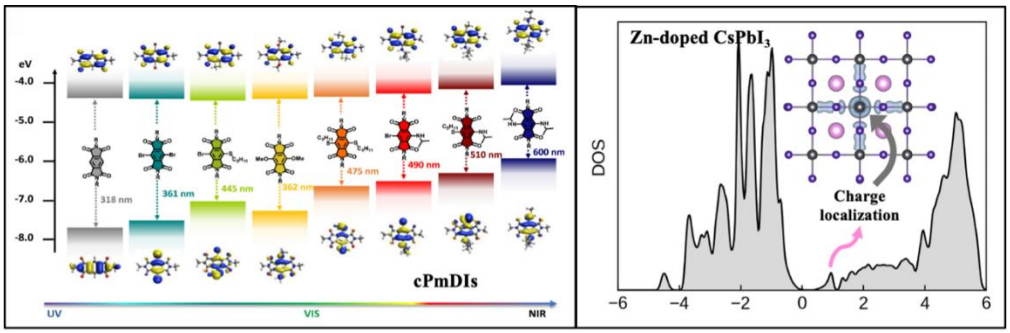


Figure 1 Tunable triplet emission in cPmDIs & PL enhancement in Zn-doped $CsPbI_3$ PNC.

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Different Water Architecture Diversifies the Catalytic Activity in Two Deceptively Similar Cytochrome P450 Isozymes

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Abstract

Cytochrome P450 (CYP450) enzymes are ubiquitous in nature, and they catalyze a plethora of biologically relevant reactions in all sorts of biological kingdoms. It uses molecular oxygen and inserts it into the incoming substrate during oxidation of the substrate [1]. Among several members of the Cytochrome P450 enzymes, CYP1A1 and CYP1A2, are pivotal in the bioactivation of polycyclic aromatic hydrocarbons (PAHs), converting them into carcinogenic metabolites [2]. Although both enzymes exhibit structural adaptation to bind PAHs and possess very similar protein structures, they show differential reactivity with α-naphthoflavone (ANF), a known CYP1 family inhibitor. CYP1A1 demonstrates minor metabolic activity toward ANF, while CYP1A2's reaction is almost negligible [3]. To investigate the mechanistic underpinnings of this selective metabolism, we perform molecular dynamics (MD) simulations and hybrid quantum mechanics/molecular mechanics (QM/MM) calculations, examining structural dynamics and electronic factors within the active sites of CYP1A1 and CYP1A2. The MD simulation of both enzymes in the presence of the ANF shows different water organization in the two enzymes. The CYP1A1, which shows metabolic activity, forms an organized water channel stretching from the ANF to the heme iron-oxo, enabling substrate oxidation via the Grotthus mechanism. While such organization was missing in CYP1A1 which is the root cause of the loss of the activity. The study provides a mechanistic insight that could help to design selective CYP1 inhibitors, contributing to strategies for mitigating PAH-related carcinogenicity by fine-tuning enzyme specificity.

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Molecular Dynamics Investigation of Conotoxin Pl14A Binding and Inhibition Mechanism on Kv1.6 Potassium Channel

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Conotoxins are peptide toxins which are found in marine cone snails and they inhibit ion channels with high affinity and selectivity. Pl14A is a conotoxin belonging to the J-superfamily, is one of a few conotoxin that can inhibit two type of receptors, the Kv1.6 subtype of voltage-gated potassium channels as well as nicotinic acetylcholine receptors. In this work, we use molecular dynamics simulations to clarify the mechanism of inhibition and structural interactions between pl14a and the Kv1.6 channel.Our study reveal that Pl14A binds stably in the extracellular vestibule of Kv1.6, engaging key residues within the selectivity filter and turret region through a combination of electrostatic and hydrophobic contacts. The peptide's basic residue, mainly arginine residues and putative dyad motif LYS18 and TYR19 , are implicated in its subtype specificity and pore-blocking activity. Structural analysis and free energy calculations provide a quantitative view of the conformational changes in both the peptide and the channel which supports a 'lid-like' blockade mechanism with binding energy of -17.5kcal/mol. These findings help us to understand the modulation of Kv1.6 channel by conotoxin Pl14A and offer insight for designing selective peptide inhibitors with therapeutic potential against Kv1.6 related pathologies.

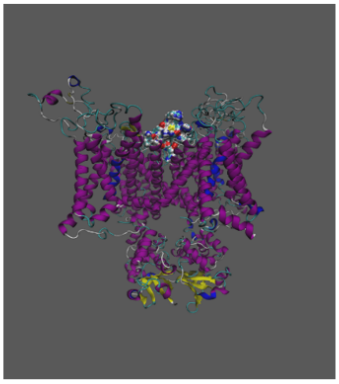


Figure 1. A molecular visualization of Kv1.6 channel and Pl14A (space-filling model) interacting within the pore region.

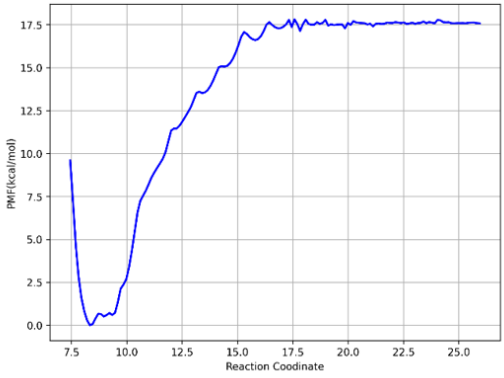


Figure 2. Graph depicting the potential of mean force generated through umbrella sampling analysis.

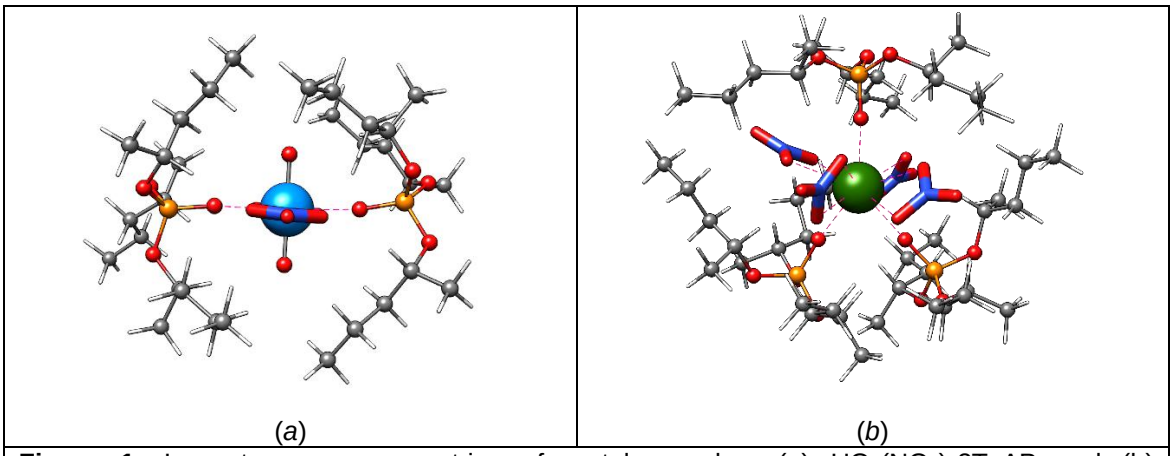
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Effect of Branching of Tri-amyl-phosphate on Extraction of Th and U

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To address the experimentally observed effect of a series of trialkyl phosphates with varied branching on the extraction of Thorium and Uranium(*e.g.*, TAP, TiAP, T2MBP, TsAP).[1,2] Density Functional Theory (DFT) has been applied to get complexation energies in order to understand the branching effect on the metal ligand interaction of their respective thorium and uranium complexes. Ligand conformers were sampled using CREST and GOAT at the GFN2-xTB level and optimized with DFT. Metal complexes were preoptimized in the Turbomole 7.3 program[3] and re-optimized in the ORCA 4.2.1 software program[4] at the RI-BP86-D3BJ/def2-TZVP-ZORA level with SARC basis sets for U, Th. Minima were confirmed by frequency calculations, and solvent effects (*n*-dodecane) were included via C-PCM single points. Complexation energies were analyzed by EDA in the ADF program[5] at the BP86-D3BJ/TZ2P-ZORA level, and electronic structures were further examined by NBO 6.0.[6]



(*a*) (*b*)

Figure 1: Lowest energy geometries of metal complexes(a) $UO_2(NO_3)_2$2TsAP and (b) $Th(NO_3)_4$3TsAP.color code: Red is oxygen, Dark Blue is nitrogen, Grey is Carbon, White is hydrogen, Green is Thorium, and Light blue is Uranium.

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Variational Excited State Density Functional Theory Vs Time-Dependent Density Functional Theory for "Difficult" Excited States

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Accurate modeling of electronic states is essential for understanding photophysical properties and designing new materials. Within density functional theory (DFT), time-dependent DFT (TDDFT)[1] is widely used to study excited states. However, TDDFT struggles to provide a correct description of certain excited states, such as, charge-transfer (CT)[1] excitations, and inverted singlet–triplet (INVEST)[1] gaps. In contrast, variational excited-state DFT (eDFT) performs remarkably well for the cases where TDDFT struggles. In this study, a general framework will be presented for comparing TDDFT and eDFT excitation energies. This framework will be applied to the INVEST and the CT excited states using a wide variety of functionals. Our study enables decomposition of excitation energies obtaind from TDDFT and eDFT into orbital energy difference, kernal contribution and orbital relaxation. Our analysis reveals that the superior performance of eDFT over TDDFT correlates directly with the interplay among these decomposed contributions.

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Theoretical Chemistry Symposium
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Geometry-Dependent Phase Behavior of Confined Water: Insights from Slit-Pore and Cylindrical Confinements

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We investigate the thermodynamic and structural properties of water under strongly hydrophilic nanoscale confinement using the monatomic water (mW) model [1]. Molecular dynamics simulations in LAMMPS were performed for slit-pore separations ($H = 8.5 - 70$ Å) and cylindrical radii ($R = 10 - 50$ Å) across 100–350 K. Water–wall interactions were modeled via a Lennard-Jones 9-3 potential, with water described by two- and three-body Stillinger–Weber potentials. Properties including density, enthalpy, potential energy, entropy, specific heat capacity, structural dynamics, and phase transition temperatures exhibit strong dependence on confinement geometry and surface interaction strength [2-3]. While slit pores display oscillatory variations in freezing temperature (T_f) with pore size, cylindrical pores show a smoother increase, with stronger hydrophilicity consistently elevating T_f relative to bulk water [Fig. 1]. Notably, small pores (H ≤ 20 Å, R ≤ 10 Å) show higher solid-phase density than liquid, deviating from bulk behavior. Hysteresis in density, enthalpy, potential energy, and entropy, along with oscillatory specific heat and abrupt order-parameter changes, indicate first-order phase transitions and diamond-like crystallization. These findings elucidate how confinement geometry modulates water's phase behavior, offering fundamental insights into nanoscale superhydrophilic environments.

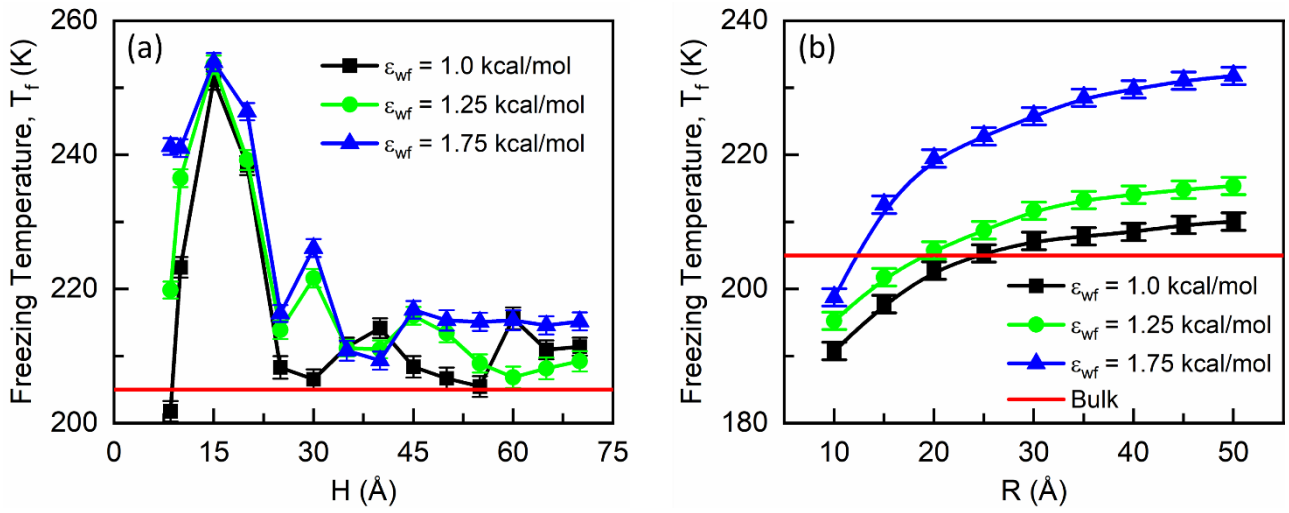


Figure 1 Freezing temperature as a function of pore size at $\boldsymbol{\varepsilon_{wf} = 1.0}$, $\boldsymbol{1.25}$, and $\boldsymbol{1.75\ kcal/mol}$ for (a) slit-pore and (b) cylindrical-pore confinements.

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Insights on the Activation of Small Molecules by Borylene and Their Electronic Structure Analysis

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Non-metal-based small-molecule activation, particularly via main-group elements, is exemplified by the CAAC-stabilized borylene CAAC–B–$N(SiMe_3)_2$. Computational studies reveal two distinct interaction modes with two types of small molecules. Type A substrates (e.g., CO, NO^+, C_2H_4) engage in pronounced donor–acceptor interactions, characterized by electron donation into the vacant p-orbital of boron and concomitant π-backdonation from the borylene fragment. In contrast, Type B substrates (e.g., CH_4, H_2, C_6H_6) primarily undergo π-backdonation into their respective σ* orbitals. These findings underscore the remarkable versatility of low-valent boron species in mediating small-molecule activation, positioning them as compelling alternatives to traditional transition-metal-based systems.

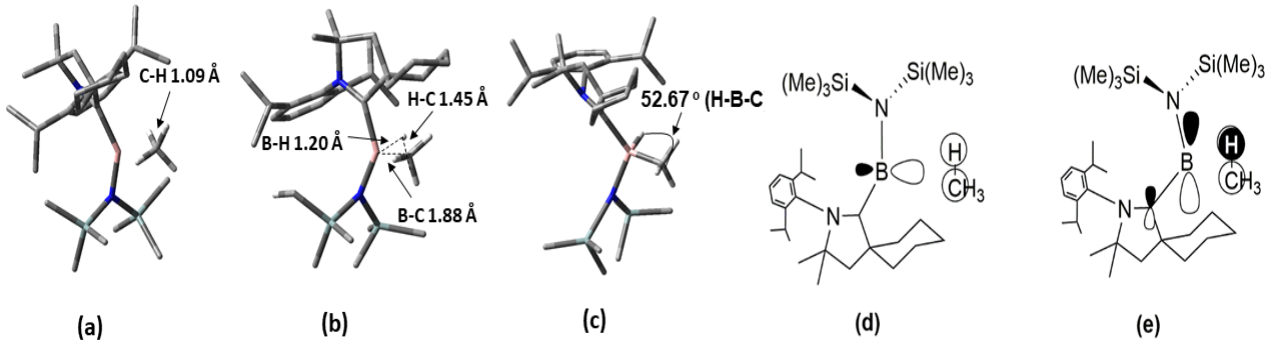


Figure 1 Calculated transition state for the activation of **CH_4**, intrinsic reaction coordinates showing the transitioning path (a) reactant (b) Transition state (c) product [H-B-C bond angle °] (d) Primary interaction between the LUMO of bent form of **NCB(H)-CH_3** and the σ orbital of **CH_4** (e) secondary interaction between the HOMO of the bent form of **NCB(H)-CH_3** and the σ* orbital of **CH_4**. Hydrogen atoms were remove for clarity.

DFT Insights into Fe–Ni–Cr Alloys: Magnetism, Stability, and Pathways to Corrosion Studies

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Multi-principal element alloys (MPEAs), particularly medium-entropy alloys (MEAs) and high entropy alloys (HEAs), attract attention for their tunable structural and magnetic properties, making them attractive for next-generation materials design. In this work, we employ density functional theory (DFT) calculations with Quantum ESPRESSO in the Schrödinger Materials Science[1] framework to study Fe–Ni–Cr alloys as a representative ternary system. Our results indicate that Fe–Ni alloys favor the BCC phase[2] at high Fe content, with Fe magnetic moments around 2.4 μB. Incorporation of Ni enhances lattice stability and slightly lowers the Fe magnetic moment to ~2.3 μB, with both Fe and Ni spins aligned ferromagnetically. Chromium, on the other hand, increases the Fe magnetic moment to ~2.5 μB and destabilizes the lattice. At low chromium concentration in Fe–Cr alloys, Cr couples antiferromagnetically with Fe while remaining xxxx ferromagnetically aligned with other Cr atoms. For ternary Fe–Ni–Cr alloys, the opposing influences of Ni-driven stabilization and Cr-induced destabilization lead to average Fe moments between 2.1–2.7 μB depending on the specific Ni and Cr concentrations. This work establishes the bulk magnetic and structural trends as a basis for ongoing studies that extend to alloy surfaces in solvent environments, with the broader aim of understanding corrosion behavior in Fe-based MPEAs with the three-dimensional reference interaction site model (3D-RISM)[3,4].

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Identifying Host-Specific Patterns in Viral Protein Sequences to Predict Host Spillover Risk in Animal and Plant Kingdoms

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Viral spillover events are a major cause of emerging pandemics; yet, their prediction remains challenging due to the combined effects of viral genetics, host adaptability, and ecological context. Existing models often focus on host or ecological traits, while sequence- and machine learning–based methods, though promising, lack a unified and generalizable framework. Here, we present SPHAK, a protein-based sequence similarity approach for assessing spillover risk and predicting viral families. This method examines protein sequences, which play a role in infection, to uncover amino acid patterns that could assist in differentiating viral hosts, potentially adding value beyond genome-level analysis. Applied to influenza datasets, SPHAK successfully detected spillover-associated protein signatures across multiple pandemic-relevant subtypes, including H1N1, H3N2, and H5N1. These results demonstrate SPHAK's accuracy and broad applicability across both animal and plant viruses, highlighting its potential as a practical tool for early warning and targeted surveillance to strengthen pandemic preparedness.

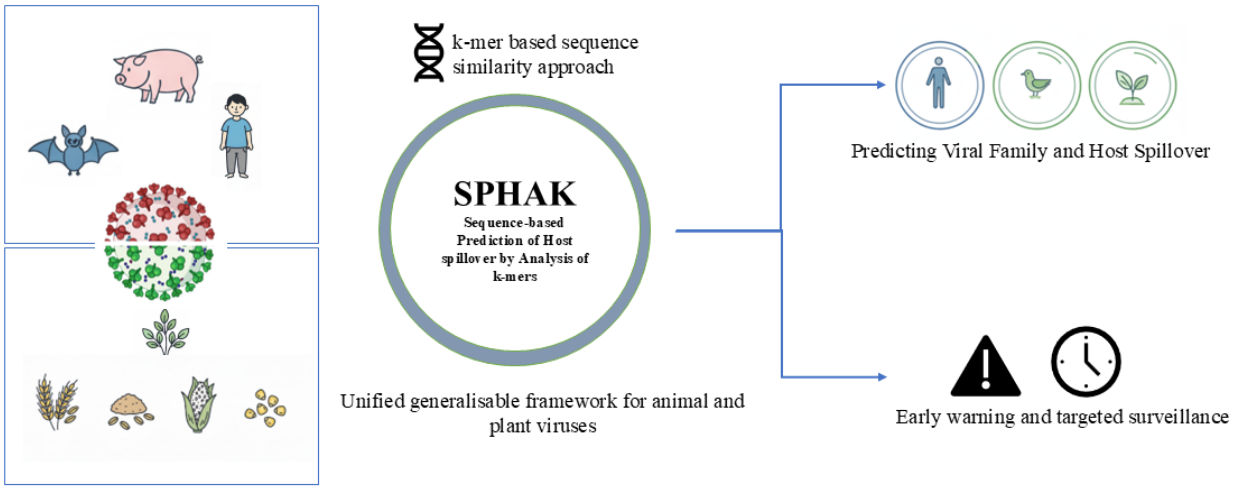


Figure 1 Conceptual overview of SPHAK

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Exploring the magnetic behavior of {Ln2} Single Molecule Magnets with diverse bridging ligands. Synthesis and theoretical Insights

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The magnetic properties of dinuclear lanthanide complexes arise from interactions between the two metal centers, often leading to cooperative effects that define their single-molecule magnet (SMM) behavior. Among the various factors influencing their energy barriers, magnetic exchange interactions are most significant.[1] The dimer geometry—particularly the spatial arrangement of the metal centers and the nature of the bridging ligands—strongly affects the overall magnetic response.[2] In this work, eight dihalide-bridged Dysprosium(III) complexes with F–, Cl–, Br–, and I– bridges, known for their large energy barriers, were selected for ab initio investigation. To further elucidate the role of di-μ-halide bridges and the co-ligands/terminal ligands, twelve additional model structures were generated by systematically substituting the halide ions within the parent complexes. These computational studies aim to rationalize how the donor strength and nature of the halide bridges modulate the magnetic exchange interactions and anisotropy in dinuclear Dy(III) systems. Additionally, we successfully synthesized a series of paddle-wheel-type {Ln_2} complexes (Ln = Tb, Dy, Ho, and Er), in which carboxylate bridges facilitate magnetic exchange. The nature of these interactions influences the overall magnetic properties.

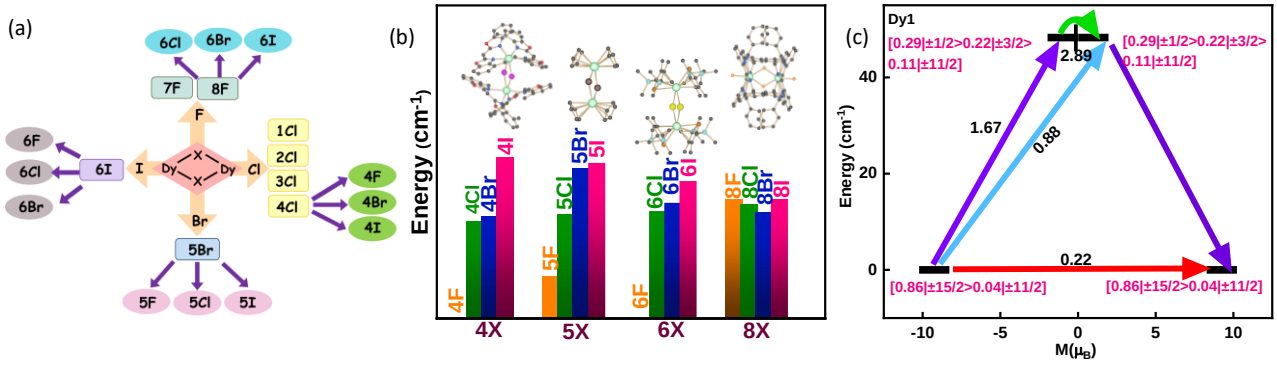


Figure 1 (a) Schematic representation of the design of model complexes from the parent complexes, and their comparitive energy barriers (b). (c) Energy barrier diagram of {Dy_2}.

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Design princples for synthesis of Phosphenium cation in H_2 splitting

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Phosphorus-based species have emerged as promising candidates in metallomimetic catalysis owing to their ability to switch between the P(III) and P(V) oxidation states[1,2] This redox flexibility, facilitated through rehybridization at the phosphorus center, can be enhanced by embedding rigid pincer ligands around the P(III) core. So far, the only ligand framework reported so far for hydrogen activation is the phosphenium cation supported by a 2,6-bis(o-carborano)pyridine backbone (Fig. 1).[3] Despite this advancement, a comprehensive mechanistic understanding of H_2 splitting using phosphorus pincer complexes remains lacking. Addressing this gap is critical not only for elucidating the underlying principles of reactivity but also for guiding the rational design of new phosphenium complexes with improved efficiency for hydrogen activation. This work aims to establish these design principles by investigating the fundamental features that govern H_2 splitting in phosphorus-based pincer systems, thereby broadening their potential application in catalytic hydrogenation and energy-related transformations.

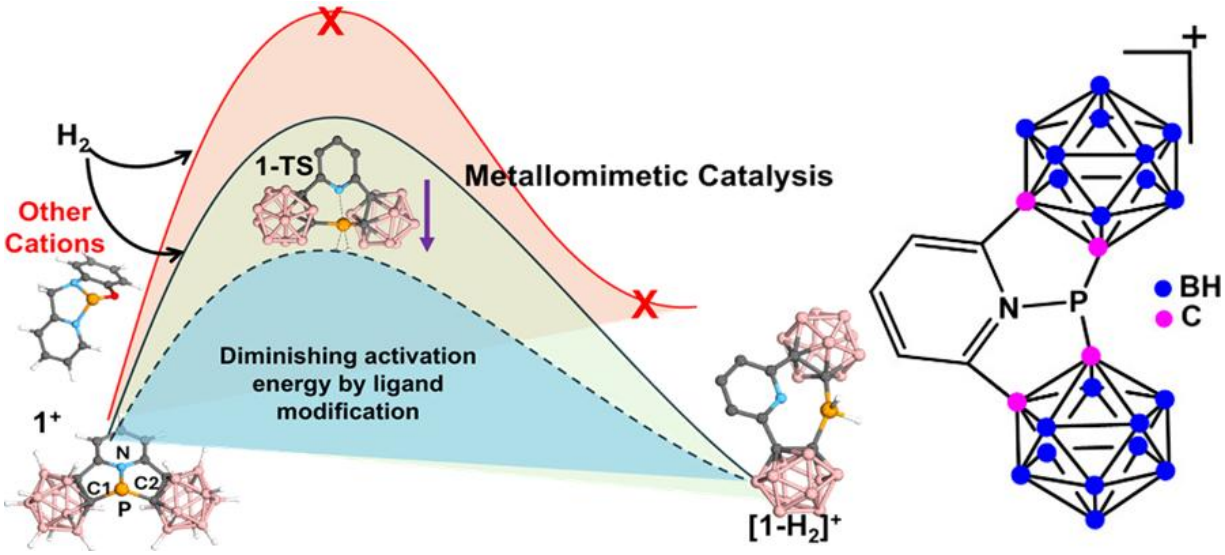


Figure 1 Reduced activation energy barrier with ligand modification for the pincer complexes.

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

Design of Multifunctional Metal-Free Two-photon Absorbing Photosensitizers for ROS Generation and Fluorescence Bioimaging

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Photodynamic therapy (PDT) has numerous advantages over conventional medicines. It has drawn a lot of attention especially in the treatment of cancer. In two-photon PDT (TP-PDT), two photons are absorbed that assists greater tissue penetration with less interference from tissue fluorescence. Because of the strong two-photon absorption cross section and lower toxicity than traditional metal-based photosensitizers, metal-free photo-sensitizers have also gained popularity in recent years. For their biomedical applications, it is vital to develop multifunctional metal-free photosensitizers with fluorescent bioimaging properties to function as Type I and Type II photosensitizers. On introducing fluorescence to such photosensitizers via structural conjugation they can be used as fluorophores for precise cell localization and real-time tracking. In this study, we theoretically investigated the reactive oxygen species (ROS) generation and fluorescence bioimaging properties of a series of dibenzothioxanthene imide (DBAI) derivatives.

The effect of helicene rings and thionation of naphthalimide framework of DBAI on the fluorescence and ROS generation is also studied. In addition, the effect of various aromatic rings orthogonal to the naphthalimide framework on the above properties is also examined. The analysis of the results showed that the above derivatives can function as potential fluorophores for bioimaging and reactive oxygen species generators. Further, the molecular docking of designed photosensitizers is studied with apoptosis promoting proteins, Fas and Fas-ligand (Fasl) that showed strong binding affinity with the proteins facilitating apoptosis.

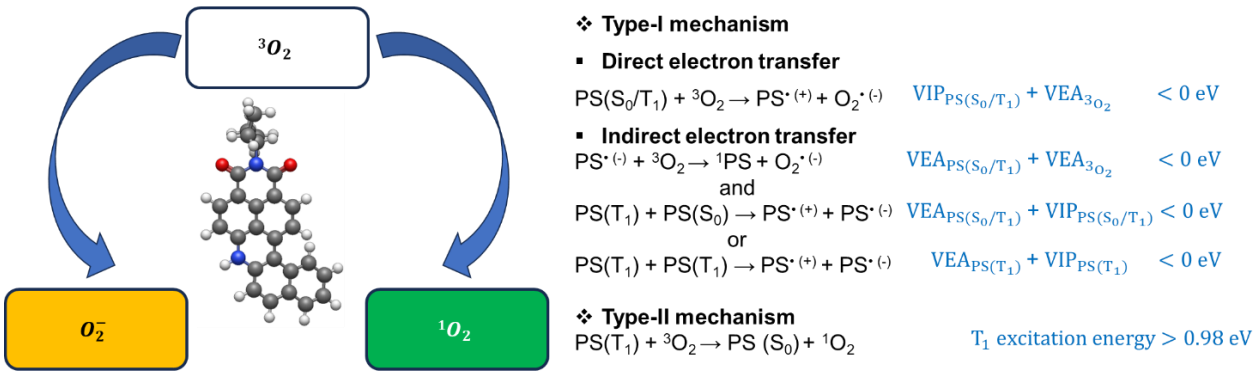


Figure 1 A schematic illustration of DBAI as duel mechanistic ROS generator.

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2. Vivek, C.N. Ramachandran, **2025** (Manuscript submitted)

Bridging Structure and Dynamics: The Pathway of Lithium Ions in Highly Concentrated Electrolytes

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Lithium-ion (Li-ion) batteries are highly efficient for rechargeable energy storage, yet their use is limited by challenges like inadequate thermal stability, slow charging, and short lifespan. To address these issues, researchers have developed highly concentrated electrolytes that incorporate lithium salts and organic additives. While these innovations improve thermal stability, conductivity remains a concern. Compatibility between salts and additives is crucial for optimizing the dynamics of these mixtures. Therefore, a robust experimental approach is essential to understand electrolyte performance based on component interactions. Our in-depth computational analysis investigates various structural and coordination factors, allowing us to track lithium ion migration through hopping and diffusion processes effectively. This understanding reveals how lithium ions traverse the solvation shell created by anion and additive molecules, and offers vital information about the competition between lithium ions for coordination with sulfone and anionic oxygen. The insights gained here pave the way for more accurate performance estimations of electrolytes, fostering advancements in energy storage technologies.

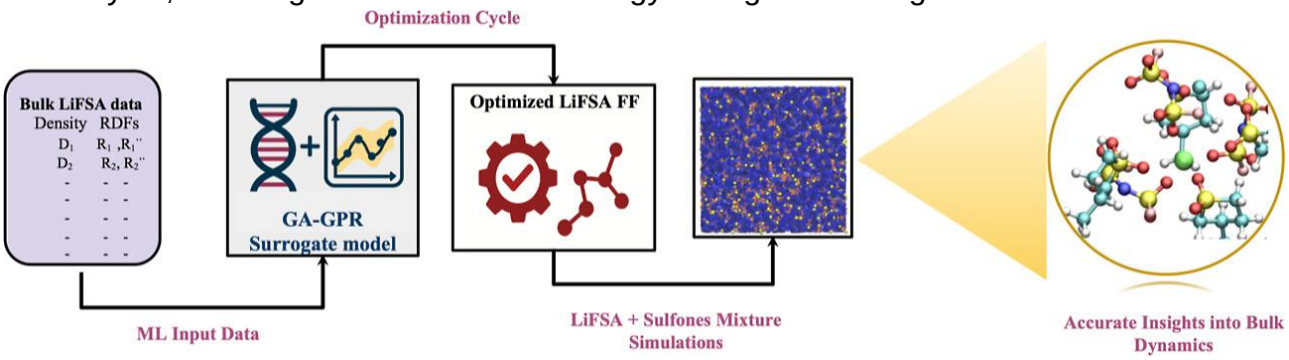


Figure 1 A schematic representation of the process followed to study the bulk dynamics.

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Theoretical Chemistry Symposium
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Design of Workflows for Accelerated Solvent Screening for CO_2 Capture: A Hybrid DFT-AI/ML Approach

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The design of efficient solvents is critical for addressing climate change by enabling effective gas separation in industries (e.g., CO_2 capture and utilization) like power generation, natural gas processing, and wastewater treatment. Solvents are also vital in pharmaceutical synthesis and energy storage. The most commonly solvents for CO_2 capture include amines and their blends (phase-separating solvents), deep eutectic solvents and ionic liquids[1]. Traditional solvent screening methods which rely heavily on experiments are not just slow but also expensive, necessitating advanced computational approaches. The current study integrates the first principles density functional theory (DFT) and Artificial Intelligence (AI) with the experimental data to accelerate the design of novel solvents for efficient CO_2 capture and utilization. The integration of AI is revolutionizing solvent discovery by combining quantum chemical (DFT) descriptors, molecular properties (via. solvation and transfer free energies, Log S, and Log P), and empirical data into predictive frameworks. A variety of classical ML algorithms, along with deep learning approaches, are used to accurately predict solvent-CO_2 interaction energies and thermodynamic parameters[2]. Machine learning models further analyze large chemical datasets to identify top performing candidates, while generative AI explores novel molecular compositions optimized for selectivity and lower regeneration energy[3]. These data-driven approaches also reveal key molecular factors influencing CO_2 affinity, enabling more rational and targeted solvent design. The hybrid DFT–AI/ML pipeline supports high-throughput virtual screening, evaluating thousands of solvent candidates in months rather than years. We explored solvation databases, including MNSol-2012[4], AqSolDB[5], and Combisolv(QM and EXP)[6], to which yielded extensive datasets of solvation and hydration free energies, and Log S values derived either from empirical methods or computational studies. These datasets are being curated to extract key insights for developing a novel pipeline (which employs a combination of structure based screening, DFT level analysis and use of advanced AI/ML tools like NLPs and transformers) that accelerates solvent design purely based on physicochemical properties and geometric features. By reducing reliance solely on empirical testing, this strategy minimizes costs and material waste, providing a scalable, sustainable, and intelligent framework for solvent innovation in CO_2 capture, catalysis, green chemistry, and materials science.

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Theoretical Chemistry Symposium
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A Molecular Dynamics Study on the Interaction of Mn^{2+} Based Contrast Agent with Human Serum Albumin

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Magnetic Resonance Imaging (MRI) is a non-invasive technique for diagnosing and detecting early cancer. The MRI technique injects a metal-centred complex called Contrast Agent (CA) into the patient to enhance the image. Inside the body, the CA agent acts as a tiny magnet, thereby enhancing proton relaxation of the water molecule. Around the globe, 40-50% of the MRI examinations use a CA agent. One of the widely used CAs is Gadolinium-Based Contrast Agent (GBCA). However, recent studies reveal that the toxic free metal ion Gd^{3+} released by GBCA caused Nephrogenic Systemic Fibrosis[1] (NSF) and Gadolinium Deposition Disease[2] (GDD) due to numerous exposures. Therefore, there is a demand for an alternate non-toxic contrast agent that has high stability and high relaxivity. As an alternative, Mn^{2+} based CA emerged as a potential replacement in recent years. Our study focuses on the interaction of Mn^{2+} based CA, which consists of one inner sphere water molecule with various biological macromolecules through classical molecular dynamics. In this context, we have first performed classical modelling of the Mn^{2+} based CA, which can reproduce the ion to oxygen distance (IOD) and residence time of the inner sphere water molecule. Further simulations were explored, using the Human Serum Albumin (HSA) protein, to understand the interaction of the Mn^{2+} based contrast agent. This study found that a non-polar side arm in the CA agent causes stronger binding with HSA, leading to longer rotational correlation time for the CA.[3] We have also observed the effect of the presence of HSA on the hydration sphere of the complex. From our study, the dynamic properties of the CA in the presence of a biological system may assist in the future development of a novel Mn^{2+} based contrast agent.

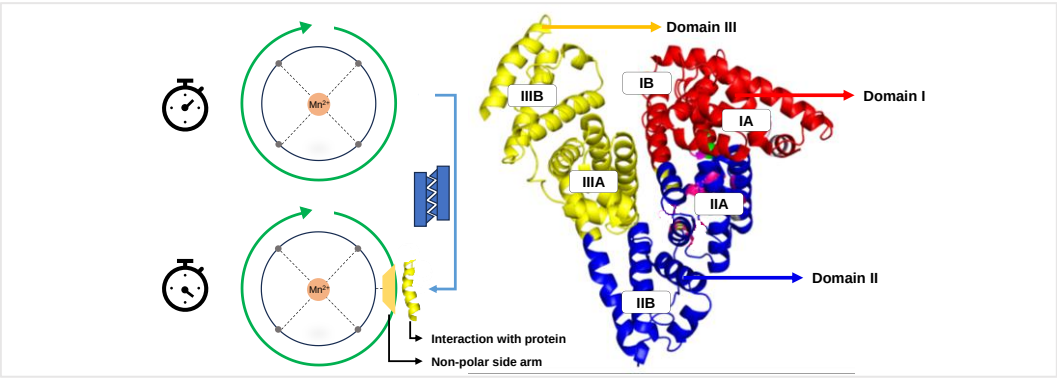


Figure 1 Interaction of Mn^{2+} metal complex with HSA resulting increased rotation correlation time.

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Oriented External Electric Field and $[Ga_4L_6]^{-12}$ metallocage

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Supramolecular catalysis within confined environments, such as the $[Ga_4L_6]^{-12}$ metallocage, offers remarkable control over reaction selectivity in processes like dienol hydrogenation.[1,2] Previous work has established that steric confinement plays a crucial role in dictating the final reaction products. However, the distinct contribution of the cage's powerful internal electric field to catalysis and selectivity remains to be explicitly quantified. This study proposes a computational investigation using density functional theory (DFT) to isolate and evaluate the electrostatic component of this catalytic effect. We have calculated the intrinsic electric field within the original host-guest complex. Subsequently, the metallocage is removed from the model, and an oriented external electric field (OEEF) that mimics the properties of this internal field will be applied to the uncaged reaction system. The complete reaction energy profile for the hydrogenation of 2,4-hexadiene-1-ol is computed under this OEEF. The central goal is to compare the results from these OEEF calculations with the established DFT data for both the fully caged and the uncaged reaction pathways. By decoupling these effects, we aim to determine if an electrostatic environment alone can replicate the catalytic control imparted by the complete supramolecular cage. The anticipated findings will provide fundamental insights into the mechanisms of confined catalysis, paving the way for the rational design of new catalysts where electrostatic and steric parameters can be independently tuned.

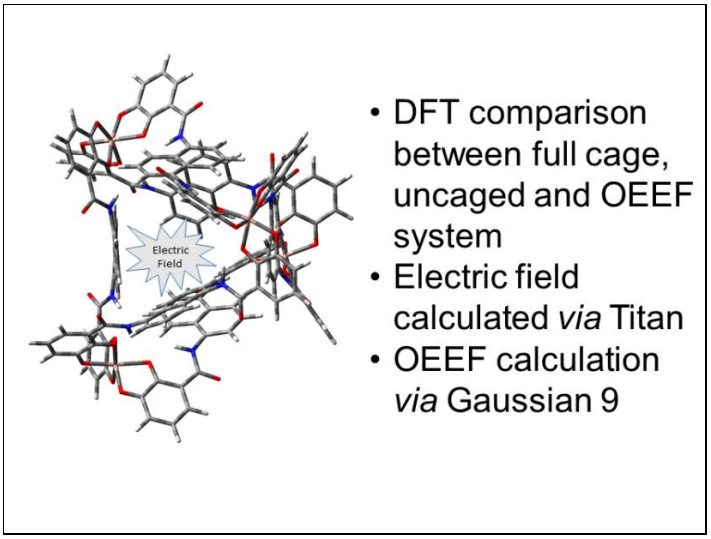


Figure 1: $[Ga_4L_6]^{-12}$ metallocage

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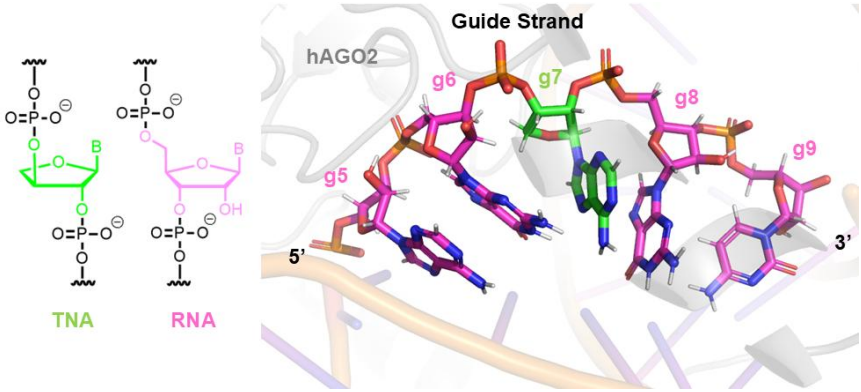
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Structural and Functional Effects of TNA Modifications on RNA Interference: Insights from the Molecular Dynamics Simulations

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RNA interference (RNAi) mediated by small interfering RNAs (siRNAs) is a powerful tool for post-transcriptional gene silencing.[1] Therapeutic efficacy of siRNAs relies on chemical modifications that resolve obstacles like nuclease susceptibility, immune system activation, and off-target effects.[2] Notably, α-(L)-threofuranosyl nucleic acid (TNA) modification confers unique advantages, arising from its shorter 3′−2′ backbone linkage compared to natural DNA and RNA.[3] RNAi activity of TNA modified siRNA is position-dependent, and modification is tolerated widely except at position 2 of the guide strand (g2) and position 11 of the passenger strand (p11).[3] We investigated the position-dependent effects of TNA modifications at g1, g2, g7, g10 of guide strand and p11 of passenger strand in siRNAs bound to human Argonaute2 (hAGO2) using molecular dynamics (MD) simulations.[4] We optimized force field parameters for the TNA modified base, and carried out 1 μs MD simulations for all the systems. Results showed that the overall stability of hAGO2–siRNA complexes was preserved, with the PAZ domain showing the highest flexibility and the MID domain remaining rigid. TNA substitution induced a sugar pucker shift from C3′-endo to C4′-exo and caused local disruptions at g2 and p11, consistent with their reported intolerance toward RNAi. In contrast, g1, g7, and g10 maintained stable non-covalent interactions and enhanced MID–PIWI domain correlations, indicative of favourable allosteric coupling. These results reveal the structural basis of position-dependent tolerance to TNA and provide insights for rational siRNA design with improved stability and specificity.



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Theoretical Chemistry Symposium
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Quantum Kinetic Modeling of Singlet Oxygen Generation in Heavy-Atom-Free Photosensitizers

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Singlet oxygen ($^1O_2$) generation is a key photophysical process driven by intermolecular energy transfer (EnT) between a photosensitizer and molecular oxygen. Accurately evaluating the kinetics of this process remains a major challenge. In this study, we present a streamlined computational protocol to estimate the EnT process using an adaptation of classical Marcus theory. This approach enables the determination of free energy barriers and provides qualitative insights into model performance when benchmarked against experimental data for diverse organic chromophores. Complementary excited-state analyses further reveal the role of higher electronic states and their interrelationships. Overall, this protocol offers a simple computational framework for calculating the kinetics of singlet oxygen generation, making it accessible for straightforward application in molecular photosensitization studies.

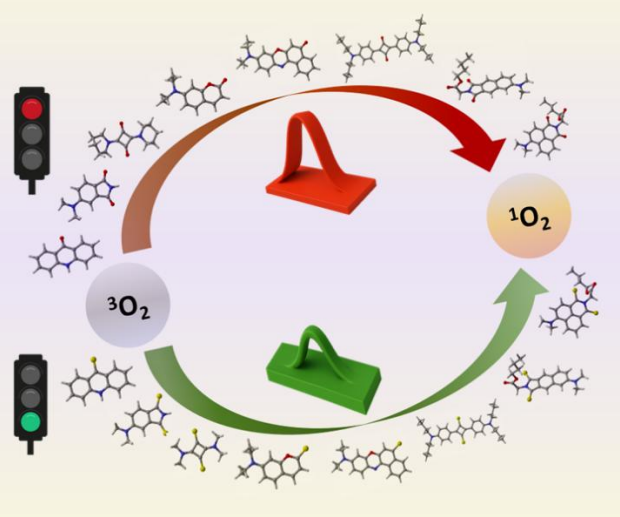


Figure 1 Mechanistic overview of singlet oxygen generation in photosensitizers

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Valence Isomerism in Biological Iron-Sulfur Clusters

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Iron-Sulfur clusters are vital for electron transfer and catalysis of biochemical processes in all forms of life, from bacteria and plants to animals.[1] They are challenging to study due to their core's (Fe_4S_4) complex electronic structure and high density of spin states. However, both of these factors are considered key to their rich chemistry.[2] Iron–sulfur clusters in proteins often exhibit antiferromagnetic coupling, where individual iron centers couple through bridging sulfides to yield a net low-spin ground state.[3] In the widely used *pairs-of-pairs* model for Fe_4S_4 clusters, the four irons form two strongly antiferromagnetically coupled Fe–Fe pairs, allowing multiple valence isomers depending on how charges are distributed across the pairs. For instance, a mixed-valence Fe(II,III) pair of high-spin ions with spin S = 9/2 and a ferrous Fe(II,II) pair of spin S = 4 are coupled antiferromagnetically to give an overall low-spin ground state (S = 1/2), which exhibits a characteristic EPR signal.[4] In the case study of Fe_4S_4 cluster in [Fe-Fe] hydrogenase using MD simulations and QM/MM techniques we found that valence isomerism between $Fe^{2.5+}$ and Fe^{2+} pairs is strongly affected by the flexibility of second coordination sphere residues (Arg227 and Lys228) thereby influencing the cluster's electronic structure and potentially its catalytic properties.[5] These results are used to understand EPR observations on the enzyme. These findings highlight the interplay between valence localization, protein environment, and structural flexibility in biological Fe–S clusters.

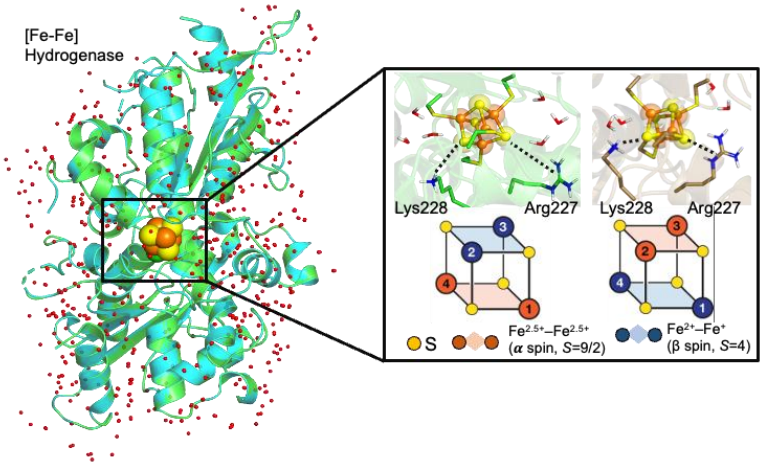


Figure 1 Schematic depiction of the valence isomers obtained by QM/MM calculations on the different configurations of Fe_4S_4 cluster.

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Exploring Metal Nanoparticles to Degrade Per- and Polyfluoroalkyl Substances

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Abstract

Per- and polyfluoroalkyl substances (PFAS) are synthetic chemicals widely used in industrial and consumer products owing to their exceptional thermal stability and unique oil- and water-repellent properties.[1-2] However, they are extremely persistent and toxic to all forms of life, including humans. The strong C–F bonds in PFAS make their degradation challenging, necessitating the search for innovative solutions. Plasmonic metallic nanoclusters (NCs) are promising in efficiently converting sunlight into chemical energy, potentially driving the chemical reactions that are otherwise impossible (i.e., thermodynamically unfavorable) under standard conditions.

Bimetallic NCs of plasmonic and catalytic metals hold great potential for improving and controlling plasmon-induced hot-carrier generation, which is valuable in plasmonic catalysis.[3-4] In this study, we use first-principles real-time time-dependent density functional theory (RT-TDDFT) to explore hot-carrier generation in noble metal NCs (Ag, Au, and Cu) with site-specific doping by both noble and catalytic metal atoms (Ag, Au, Cu, Pd, and Pt). We find that the overall plasmonic response of the nanoparticle remains largely dependent on the surface atoms. At the same time, the generation of HCs and subsequent transfer to the PFAS molecules are strongly influenced by the dopant atoms. Doping with catalytic metal atoms (Pd and Pt) significantly enhanced the DHET from NC to PFAS. This suggests a promising route to tailor plasmon formation, its decay into HCs, and transfer to PFAS, thereby achieving complete degradation by selecting appropriate dopants.

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Molecular insights into liquid-liquid equilibria obtained on use of alcohols for efficient extraction of acetonitrile from its mixtures with water

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Acetonitrile, being a xenobiotic that readily volatilizes into the atmosphere, poses a severe concern to the health of human beings and animals when it is released into the environment because it breaks apart into toxic hydrogen cyanide and acetaldehyde (Wexler 2014). Consequently, ACN is regarded as one of the essential contaminants in industrial wastewater, and its removal from water is important. Considering the toxicity of acetonitrile, molecular simulations (which are computer experiments) are a cost-effective alternative to physical experiments; and the results obtained will reduce the number of experiments to be performed to find efficient task-specific solvents for wastewater treatment. In literature mixtures of acetonitrile and water, as also mixtures of alcohols with acetonitrile and water, have been studied in single-box simulations performed in the isothermal isobaric ensemble. The novelty of this study (as compared to literature) is that it is on liquid-liquid equilibria (LLE) where, besides generating the coexistence data and computing the Gibbs free energies of transfer for acetonitrile from the aqueous to the organic phase; molecular insights obtained which characterize the features of the radial distribution function will permit us to identify efficient solvents as well as design new, novel solvents. Towards gaining molecular insights into the use of methanol or ethanol as an extraction solvent to remove acetonitrile from its mixture with water, we have performed three-box GEMC simulations to model LLE using the molecular simulation technique pioneered by Keasler and co-workers. The three thermodynamically connected boxes represent the water-rich aqueous phase, the organic-rich phase, and a dummy vapour box containing helium atoms. The third box increases the rate of particle transfers between the two liquid boxes. Total number of molecules for the entire 3-box system combined contains 1000 water, 300 acetonitrile, 300 ethanol/methanol, and 50 helium molecules. Water is modeled using the TIP4P/2005 force field, whereas acetonitrile, ethanol/methanol, and helium are modelled using the TraPPE-UA force field. For ethanol as the extraction solvent at 293.15 K and 101.325 kPa, the chemical potentials of all three species in the coexisting aqueous and organic phases are in good agreement establishing equilibrium has been attained with partition coefficient of acetonitrile in the organic and aqueous phases is 5.09. The Gibbs free energy of transfer for acetonitrile is -2172.45 J/mol; the negative value confirming that the transfer to the organic phase is favourable. We also note here that the specific density of the aqueous phase is 0.937 g/cm3, and that of the organic phase is 0.807 g/cm3. Our investigations show that ethanol is a better solvent than methanol (Gibbs free energy of transfer for acetonitrile is -141.47 J/mol) as methanol is more soluble in water and to understand the underlying physics, we compare the site-site intermolecular radial distribution functions in the organic-rich phase of both the systems. For the site-site RDF of N from acetonitrile and H of the hydroxyl group of alcohol, we find in Figure 1 that first peak occurs at 1.8 Å with ethanol peak height of 3.4 being much higher than the methanol peak height of 1.65, indicating more affinity of acetonitrile towards ethanol whereas the reverse is seen in the site-site RDF (Figure 2) of N in acetronitrile with respect to the H of water. These are the

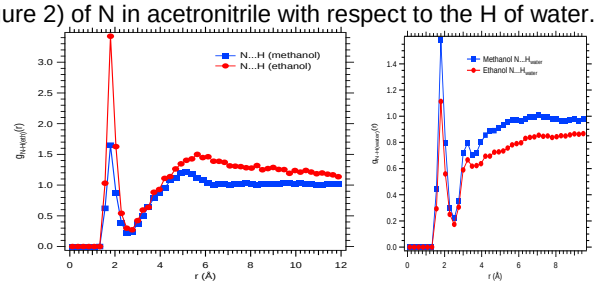


Figure1a: RDF of N in acetonitrile and H in the hydroxyl group of alcohol. 1b : RDF of N in acetonitrile and H in water

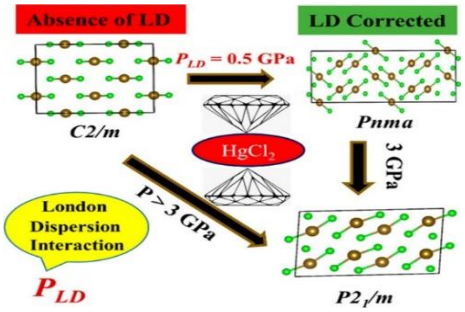
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London Dispersion Interactions Imitate Internal Pressure for Molecular Crystals

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Abstract: The packing of molecular crystals, in which the constituent molecular units have no directional forces, is primarily controlled by weak London dispersion (LD) forces. These forces assist in stabilizing the system by bringing the molecular units into the proximity of each other. The same effect is shown to be externally induced by pressure. The minimal pressure required to correctly describe the crystal structure without LD interactions (PLD) provides a quantifiable measure for the weak intermolecular interactions. LD interactions can cause phase transitions akin to external pressure in molecular solids. This attractive force acts as an internal pressure for the crystals, and therefore, the absence of LD forces creates rarefied and fallacious arrangements of molecules in solids. Most importantly, the LD forces are most crucial at ambient pressure, where its weak attractions glue the crystal. Under pressure, the molecules start packing densely, and therefore, external pressure provides a surrogate for LD forces. Only when PLD compensates for the lack of the weak intermolecular forces can the correct structure with the proper space group be obtained. At PLD, there is an abrupt change in packing as a function of pressure, which acts as a good measure of London Dispersion forces.



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Microscopic Insights into the Solvation of Stapled Peptides–A Case Study of p53-MDM2

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Water, often termed the universal solvent, plays a vital role in numerous biomolecular processes, including protein–protein interactions. These interactions are frequently mediated by water molecules, making their characterization essential for developing therapeutic strategies. One such critical complex is p53-MDM2, which is central to cellular regulation. Inhibiting the p53-MDM2 interaction remains a significant therapeutic challenge, and stapled peptides have emerged as promising candidates in this context.[1] The stapled peptides are peptidomimetics in which the side chains of two suitably positioned amino acids are covalently linked using an appropriate chemical moiety.[2] In this study, we investigate the role of water in the binding of stapled p53 peptides to MDM2 using extensive molecular dynamics simulations. Our aim is to understand how variations in the chemical nature and stapling position of the hydrocarbon cross-linker influence the behavior of water molecules surrounding the p53 peptide. We demonstrate that such modifications significantly alter the structure and dynamics of the surrounding solvent. Using rigorous entropy calculations, we rationalize the enhanced binding affinity of stapled p53 peptides compared to that of their unstapled counterparts from a solvent-centric perspective. Specifically, the entropy gain of water molecules around the stapled peptides, combined with the conformational entropy loss of the peptide, contributes favorably to binding.[3] These findings offer valuable insights into the rational design of stapled peptides and support the development of improved therapeutic inhibitors targeting the p53-MDM2 interaction.

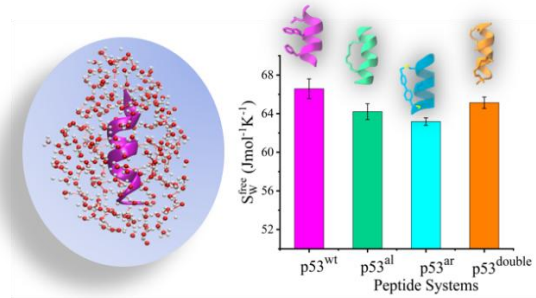


Figure: The hydration layer surrounding the p53 peptide, and the entropy of these water molecules reported in bar plot.

Keywords: Stapled peptides, MD simulations, hydration layer dynamics, Water entropy

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Comparative Dynamics of Tangentially Active Polymer Chain and Active Brownian Polymer Chain in Crowded Environments

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Abstract: Active polymers, unlike their passive counterparts, operate far from equilibrium and display complex transport and conformational dynamics. Two key theoretical frameworks— Active Brownian Polymer Chains (ABPCs) and Tangentially Active Polymer Chains (TAPCs)—capture distinct driving mechanisms: ABPCs rely on bead-level propulsion with stochastic reorientation, while TAPCs are propelled tangentially along the backbone, mimicking biological propulsion in systems such as T. Tubifex worms. While both models have been studied individually, a direct comparison in crowded and disordered environments has remained limited[1].

In this study, we use Brownian simulations to systematically contrast TAPC and ABPC dynamics in pillar arrays mimicking heterogeneous environments. Our results reveal that TAPCs exhibit intriguing conformations depending on obstacle packing fraction: spiral-like structures at low density or in free space, and reptation-like motion at high density[2,3]. These conformations lead to non-monotonic trends in dynamics and trapping as a function of packing fraction. In contrast for ABPCs, the dynamics decrease monotonically with obstacle packing fraction. of obstacles[4,5]. Interestingly, TAPCs show reduced trapping and enhanced dynamics in comparison to ABPCs in highly packed, disordered environments because of the reptile motion in the former case and coiled trapped conformations for ABPCs[6].

These findings highlight that distributing activity along the polymer backbone fundamentally alters transport compared to localized, bead-level propulsion. Beyond theoretical relevance, this comparative framework provides insights into biological navigation, intracellular transport, and the design of soft robotic agents capable of navigating complex terrains.

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Computational Insights into Enantioselective Copper-Catalysed Reductive Coupling of Alkoxy-allenes to Access 1,2-syn-Diols

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The synthesis of enantiomerically enriched complex alcohols is an attractive target in organic synthesis.[1-2] In this work, we have tried to rationalize the origin of enantio and diastereoselectivity in copper(I) catalyzed synthesis of 1,2-syn-sec, tert-diols via the reductive coupling of ketones with alkoxy allene.[3-4] Density Functional Theory (DFT) computations suggest that the reaction proceeds through a kinetically favorable 'open' Zenolate copper-alkoxy allene conformer over its E-enolate counterpart. Thereby, it facilitates syn-selectivity in the subsequent nucleophilic addition to ketone, ultimately leading to 1,2syn-sec and tert-diols. The most favorable transition state undertakes a six-membered chair configuration where the si-face of the ketone attacks the si-face of cis allene to give (R, R)diol as the major product facilitated by minimum reorganization energy and extensive noncovalent interactions.

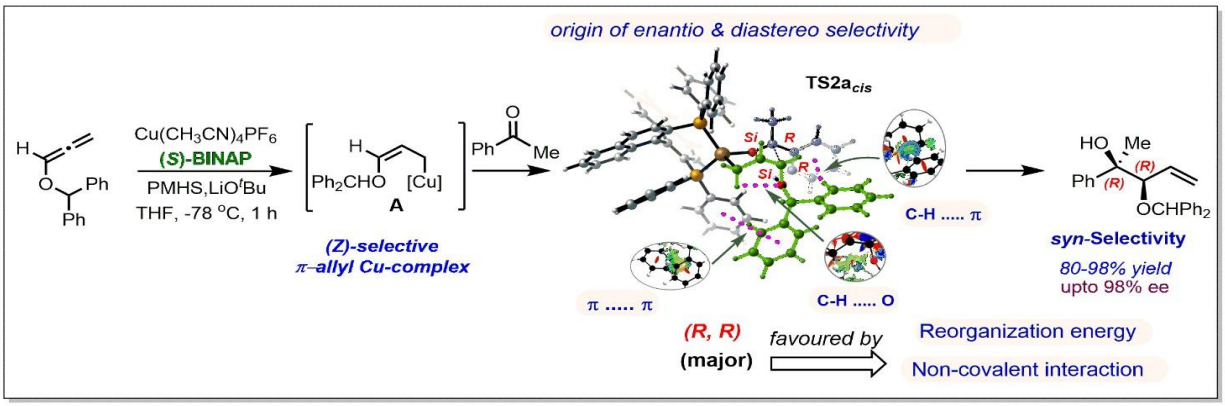


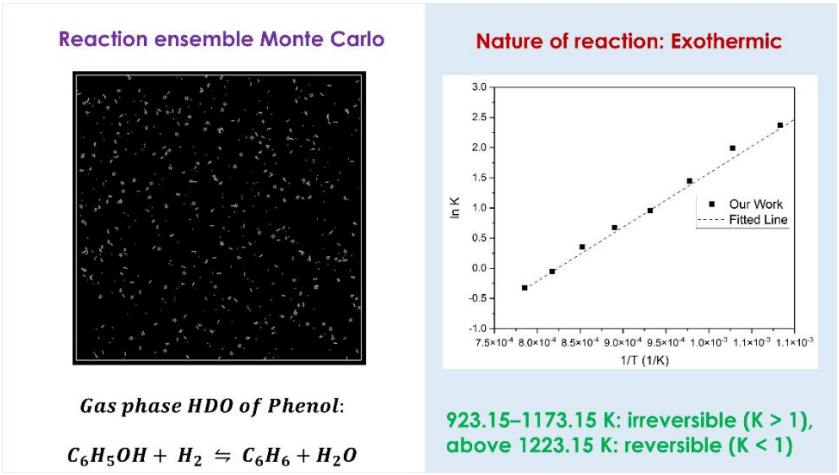
Figure 1 Cu (I) BINAP catalyzed enantio and diastereoselective allylation of ketone

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Thermodynamics of Hydrodeoxygenation of phenol to benzene: A Monte Carlo simulation study

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The reaction equilibria of the reaction of interest in this work, i.e., $C_6H_5OH + H_2 \leftrightharpoons C_6H_6 + H_2O$, (where, C_6H_5OH, H_2, C_6H_6 and H_2O represent the chemical formulae of phenol, hydrogen, benzene and water, respectively) is studied via reaction ensemble Monte Carlo (RxMC) simulations[1]. Continuous fractional component Monte Carlo (CFCMC)[2] simulations in isobaric isothermal (NPT) ensemble at 101.325 kPa and temperature range from 923.15 K to 1273.15 K are performed. All simulations start with a random configuration of 300 phenol and 300 H_2 molecules, and no benzene and water molecules. The RxMC method requires prior knowledge of the ideal-gas partition functions of all reactant and product molecules, a list of all possible chemical reactions in the system, and a suitable force field that accurately represents intermolecular interactions. DFT calculations were performed using Gaussian16® software package for each component to calculate θ_{vib}, $\theta_{rot,A/B/C}$ and D_0 (vibrational temperatures, rotational temperatures and dissociation energy or atomization energy, respectively.) for molecular partition coefficient; which is given as input to Brick–CFCMC. The geometry optimization using B3LYP level of theory with the 6-31++G(d,p) basis set was performed in case of each component to estimate θ_{vib}, $\theta_{rot,A/B/C}$ and D_0. Our simulation results show that the equilibrium mole fraction of benzene decreases with increase in the reaction temperature, demonstrating the exothermic nature of the reaction. Further, we have computed the equilibrium constant (K) at each temperature and found good agreement of ln K values with available literature data. The equilibrium constant of the reaction also decreases with increasing reaction temperature. The plot of ln K vs 1/T is a straight line and the slope of the line gives enthalpy of the reaction. The value of $\Delta H = -74.2\ kJ/mol$, which also confirms that reaction is exothermic.

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Comparative structural and functional insights into apo, active, and allosteric states of CYP3A4

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Cytochrome P450 3A4 (CYP3A4) is a key human xenobiotic-metabolizing enzyme with remarkable versatility and complexity. Its large, adaptable binding pocket enables interactions with ligands at both the active and allosteric sites, often resulting in deviations from classical Michaelis–Menten kinetics. While the Michaelis constant is commonly used to infer substrate binding affinity, it does not necessarily reflect catalytic efficiency, highlighting the multifactorial nature of CYP3A4's mechanism. This indicates that ligand binding affinity alone cannot fully explain the enzyme's conformational stability or activity.

In this study, we analyzed sequence conservation across 57 human CYP isoforms and conducted extensive molecular dynamics simulations totaling 9 µs on CYP3A4 in three distinct states: apo, active-site ligand-bound, and allosteric-siteligand-bound. These simulations were derived from a uniform experimental framework to minimize systematic bias. Our results revealed a clear hierarchy of conformational stability, with the allosteric-bound state being the most stable, followed by the active-site-bound and apo states. Notably, this stability pattern did not correlate with ligand binding affinities or intrinsic ligand conformational stabilities. Instead, the interactions between the heme cofactor and the protein showed a strong association with overall enzyme stability. These findings suggest that allosteric ligand binding stabilizes CYP3A4 by modulating heme–protein interactions, providing new insights into the structural dynamics and regulatory mechanisms of this critical enzyme.

Keywords: Cytochrome P450, CYP3A4, allosteric modulation, enzyme dynamics, molecular dynamics simulation, heme interaction.

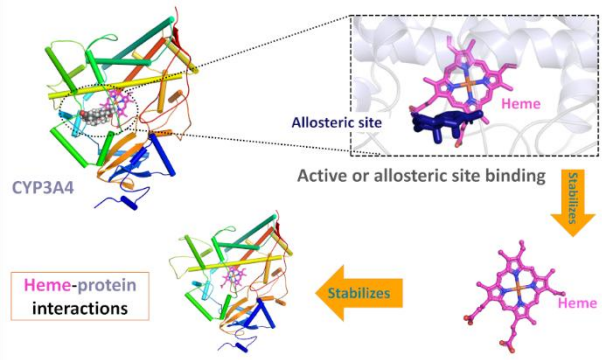


Figure 1. Summary of current work.

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UniGEN-DDI: Computing drug-drug interactions using a unified graph embedding network

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Identifying drug–drug interactions (DDIs) is essential for patient safety and treatment efficacy. While some drug combinations yield synergistic benefits, others may cause severe adverse effects, including lethality. Experimental studies provide valuable insights into DDIs but are constrained by cost and time. To address this, we developed UniGEN-DDI (Unified Graph Embedding Network for Drug–Drug Interaction), a computational model for DDI estimation. UniGEN-DDI integrates biochemical association data from DrugBank 5.1.0 and applies a combination of GraphSAGE and Node2Vec to capture diverse drug features efficiently. The model's simple yet unified design reduces computational overhead while achieving high predictive accuracy. Evaluations on balanced datasets and challenging non-overlapping splits based on drug action demonstrated both robustness and efficiency. Notably, UniGEN-DDI identified 15 previously unknown DDIs in the top 20 predictions (75% accuracy) and correctly detected 68% of unknown DDIs among the top 50 predictions, later confirmed by experimental evidence in DrugBank 6.0.

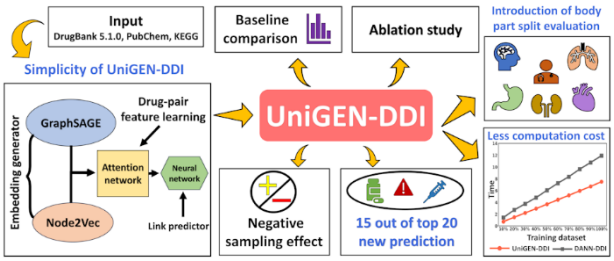


Figure 1 Summary of UniGEN-DDI.

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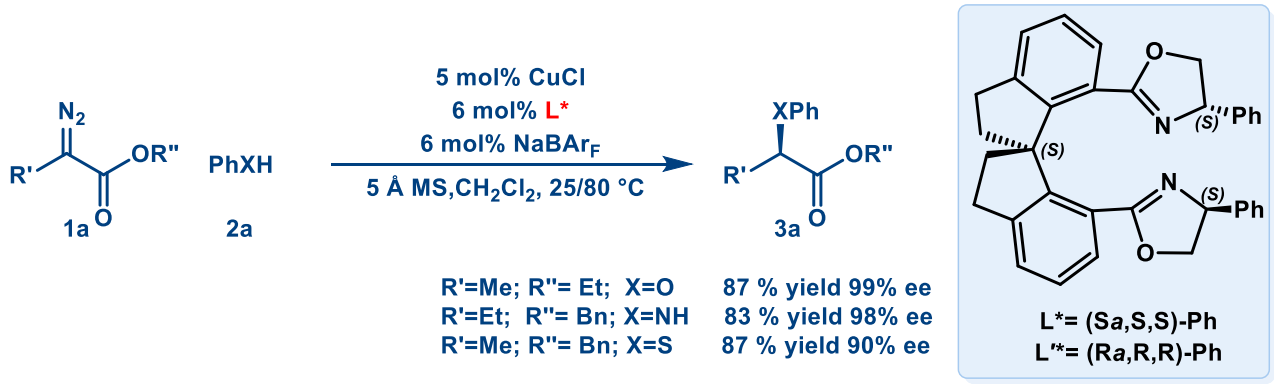
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Cu-Catalyzed Asymmetric Carbene Insertion into N–H, O–H and S–H Bonds: Challenging the Existing Mechanistic Dogma

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Cu is a versatile base transition metal that has been extensively used in various asymmetric carbene insertions for the construction of C-X bonds. Owing to its earth abundance, sustainability, and exceptional catalytic performance, Cu stands out as a particularly attractive alternative to noble metals such as Rh, Pd, Au,Ag, and Fe.[1] For the past decade, it has been believed that Cu-catalyzed asymmetric carbene insertion follows an enolate mechanism.[2] Here, we present a comprehensive mechanistic study of asymmetric carbene insertion into N–H, O–H, and S–H bonds that challenges this long-standing mechanistic proposal.[3] Our DFT and DLPNO-CCSD(T) calculations show that in all cases, the preferred route involves metal-associated enol intermediates. The study further elucidates the effect of nucleophiles on the tautomerization step: O–H and S–H insertion follow a stepwise route, whereas N–H insertion adopts a concerted pathway. A unified stereochemical model has been proposed, where the tautomerization step governs the stereochemical outcome for all three systems. Additionally, our analysis shows that monomeric Cu species are the active species, and CuL_2 species are the resting state, which is also responsible for the slight positive NLE. The research highlights the pivotal role of enol intermediates in carbene chemistry, which might be more prevalent than what is currently believed. Our study provides the first unified mechanism for Cu-catalyzed carbene insertion reactions, which will further aid in advancing catalyst design.

Scheme 1: Cu-SpiroBox Catalyzed Carbene Insertion into X–H Bond



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Mechanistic Insights into the Reduction of Molecular Nitrogen to Ammonia over Doubly Silicon-Substituted Cyclo[18]carbon

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The effect of silicon substitution on the structural stability, geometry, and electronic properties of cyclo[18] carbon (C_{18}) and its silicon-doped derivatives ($C_{17}Si$ and $C_{16}Si_2$, including isomers $C_{16}Si_2(0)$–$C_{16}Si_2(8)$) are systematically investigated the wb97xd/def2tzvpp level of theory. Among the nine possible $C_{16}Si_2$ isomers, $C_{16}Si_2(8)$, identified as the most thermodynamically stable configuration due to the maximum separation between the two silicon atoms, is selected for a detailed exploration of its catalytic behavior. DFT-based mechanistic analysis reveals that the silicon centers in $C_{16}Si_2(8)$ possess high electron density and strong orbital overlap with the antibonding orbitals of molecular nitrogen (N_2), thereby facilitating N_2 activation through the formation of stable Si–N_2 adducts. Upon successive hydrogen addition, four H_2 molecules participate in stepwise hydrogenation reactions that ultimately yield two NH_3 molecules, accompanied by the formation of a $C_{17}Si$–H_2 byproduct. Remarkably, the catalyst regeneration occurs spontaneously through an in-situ interaction between the unreacted $C_{17}Si$–N_2 species and the byproduct, leading to the formation of a $C_{17}Si$–$(NH)_2$ intermediate. These intermediate further re-enters the catalytic cycle, maintaining the continuity of the ammonia synthesis process. Overall, these results highlight the crucial role of doubly silicon-substituted cyclo[18]carbon in modulating the electronic structure, enhancing its reactivity toward nitrogen fixation, and establishing a sustainable, self-regenerating pathway for catalytic ammonia production.

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From Adsorbent to Selective Electrocatalyst: In-silico Imine-Based Ligand Engineering of CALF-20 for Electrocatalytic Ammonia Production

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ABSTRACT
Electrocatalytic ammonia synthesis is emerging as a globally compelling, sustainable alternative to the Haber-Bosch process under ambient conditions. As a result, active-site engineering has taken center stage in the development of stable and effective electrocatalysts. In this work, we report how the introduction of an imine group in the ligand backbone of CALF- 20, a Zn-based, moisture-stable MOF with high surface area, results in the formation of an N4 macrocycle for transition-metal anchoring. PBE+D3 calculations, supported by spectroscopic, ab initio molecular dynamics, and electronic analyses, identify Fe-bound modified CALF-20 as the most stable configuration among the Mn-, Fe-, Co-, Ni-, Cu-, Ru-, Rh-, Ag-, and Au- anchored within the modified CALF-20 framework. Upon modification, the d-band center shifts from −5.08 to −4.44 eV in MFe-CALF-20. Adsorption studies confirm activation of both N_2 and NO_2, reflected by bond elongation and red-shifted IR peaks. Mechanistic studies show that MFe-CALF-20 selectively facilitates NH_3 formation, exhibiting PDS values of 0.69 and 0.62 eV for the NRR and NO_2RR, respectively, while a competitive adsorption shows a clear preference over HER. Our study illustrates how functionalization tunes CALF-20 for dual application as an adsorbent and as an electrocatalyst for NH_3 synthesis and storage.

Exploring the Disruption of c-Myc–Max Dimer by Small Molecules: A Metadynamics-Based Mechanistic Study

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Our work investigates the molecular mechanisms of inhibition of c-Myc-MAX dimerization by three small molecules inhibitors, Epigallocatechin gallate (EGCG) [1], KJ-Pyr-9 [2] and 10058-F4 [3], using well-tempered metadynamic simulations. All molecular dynamics (MD) and metadynamics (MetaD) simulations, as well as free energy surface (FES) generation, were performed using GROMACS [4] integrated with PLUMED [5] plugin. The free energy surface plots were constructed along carefully chosen collective variables (CVs), including solvent-accessible surface area (SASA), number of hydrogen bonds, and interfacial salt bridges between c-Myc and MAX. The study demonstrates that each inhibitor exerts distinct effects on the free energy landscape of c-Myc-MAX dimerization, revealing specific disruption pathways and conformational changes. These insights underscore the value of computational approaches in elucidating molecular interactions and guiding rational inhibitor design against oncogenic protein-protein interactions in cancer therapy.

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Theoretical Chemistry Symposium
(TCS-2025), VMCC, IIT Bombay, India

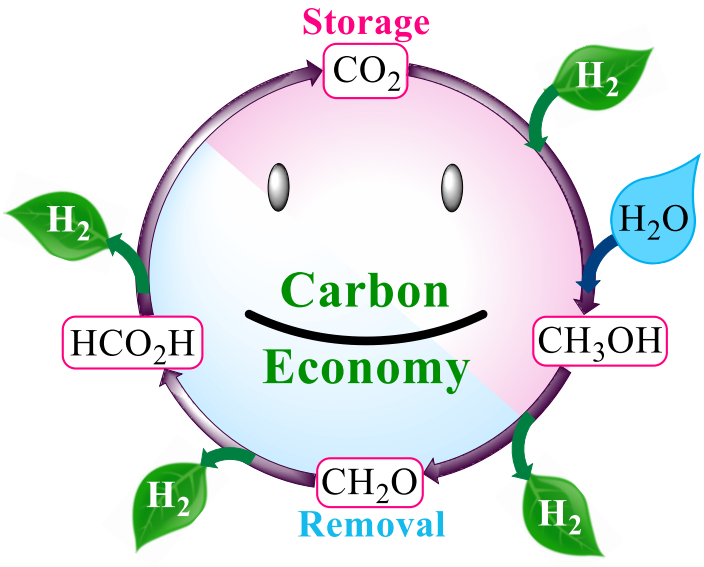
Designing Fe (II)NNN Pincer Complexes for Base-Free Green Hydrogen Production from Methanol

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Methanol dehydrogenation using earth-abundant catalysts in the absence of any additives presents a promising route for green hydrogen production in fuel cell applications. This study investigates the catalytic performance of three Fe (II)NNN pincer complexes through density functional theory calculations. The turnover frequency analysis, based on the computed free energy activation barriers, reveals that the **1c** Fe (II)NNN pincer complex exhibits better catalytic activity in comparison to **1a** and **1b** Fe (II)NNN pincer complexes. These trends are consistent with electronic structure analyses, including condensed Fukui functions, HOMO-LUMO gap evaluations, and distortion-interaction analysis, which collectively provide insight into the key electronic and structural features that enhance the catalytic performance. Notably, the study indicates that the reaction pathway remains energetically accessible in the absence of an external base, which has great implications for designing base-free catalytic systems. Moreover, the less electrophilic central metal contributes to lower free energy activation barriers under such base-free conditions, indicating potential for improved catalytic performance without the need for external base additives. Overall, this study provides a critical understanding of the structure-activity relationship, paving the way for the rational design of next-generation, sustainable catalysts for green hydrogen production from methanol.



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Solution of Generalized Operators in the Variational and Projective Quantum Framework

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Variational quantum eigensolver (VQE) provides a lucrative platform to determine molecular energetics on noisy intermediate scale quantum (NISQ) architecture. VQE relies on the construction of a wavefunction ansatz that ideally should be expressive yet sufficiently compact for NISQ realization. To address this, we come up with a robust ansatz construction protocol[1] that automatically adapts itself depending on the degree of correlation of the system through one and two parameter energy optimization, ordering and operator commutativity pre-screening. In addition to that a theoretical methodology[2] is developed to solve the generalized operators in the projective quantum eigensolver (PQE) framework, demonstrating enhanced noise resilience and accelerated convergence compared to the VQE under realistic quantum noise. By introducing lower-order generalized operators into the projective framework, our approach effectively captures strong correlation effects without the explicit inclusion of higher-order excitation terms. We have shown that this methodology leads to a substantial reduction in quantum resource demands, particularly in the number of quantum gates, thereby making it more feasible for near-term quantum hardware.

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Resource Efficient Electronic Structure Calculations via Subspace Optimization and Machine Learning: Classical and Quantum Computing Aspects

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[1]Department of Chemistry, Indian Institute of Technology Bombay

The holy-grail of electronic structure theory is solving Schrodinger's equation accurately with minimal resource requirements. While classical methods such as coupled cluster (CC) requires a higher-order polynomial scaling, its unitary variant suited for quantum computing architecture suffers from deep quantum circuits and huge number of measurements. To address such problems, we propose a general framework that assumes an adiabatically decoupled structure in the many-body operator space consisting of a *principal* and an *auxiliary* sub-part. Such a decoupling projects the effective optimization problem into an extremely lower dimensional principal manifold. Further, we establish a mathematical formalism for the reconstruction of the auxiliary parameters from the principal parameters via machine-learning[5] or analytical methods[1-4] and subsequent inclusion of these parameters into the energy function as a post-optimization correction without any major computational overhead. Our method is general in nature such that it can be incorporated across different domains such as CC or Variational Quantum Eigensolver (VQE)-like optimization protocols. The numerical demonstrations show drastic reduction in resource utilization (in terms of number of matrix operations,quantum measurements or circuit depth) without compromising the accuracy for molecular energetics.

Keywords: Quantum Chemistry, Quantum Computation, Coupled Cluster, Variational Quantum Eigensolver

References :

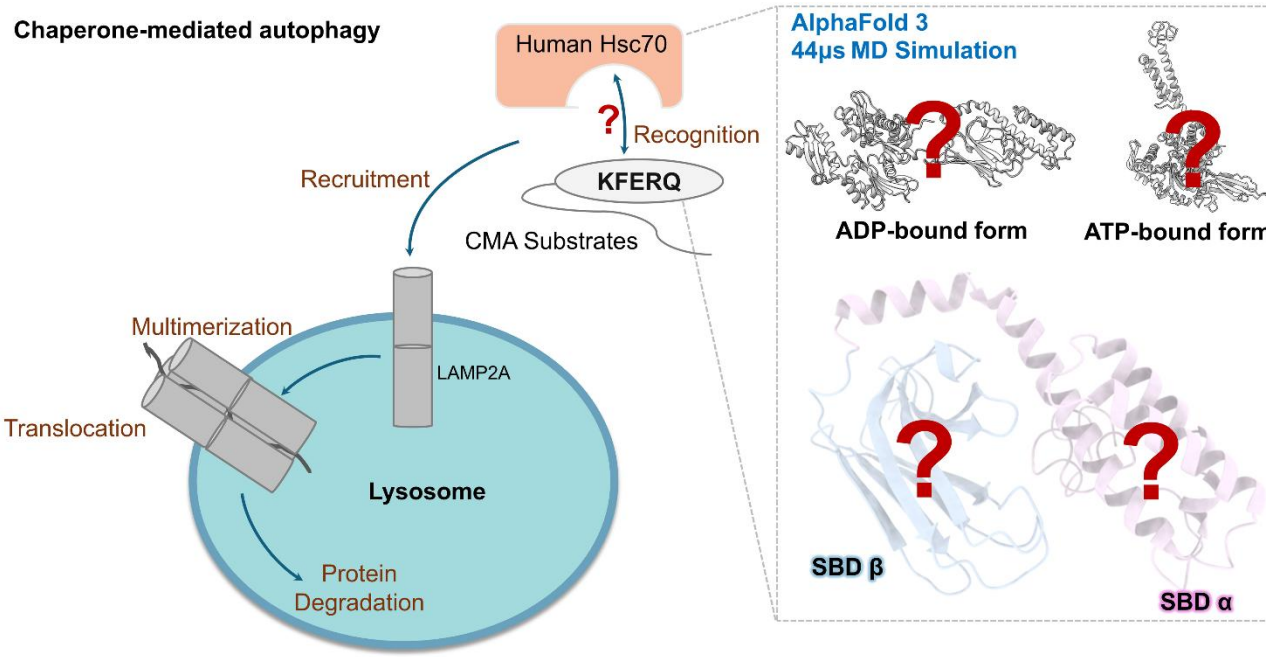
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Investigation of Hsc70 binding sites with Chaperone-mediated autophagy substrates: An integrated computational approach

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Chaperone-mediated autophagy (CMA) selectively targets dysfunctional proteins for degradation through the recognition of KFERQ-type motifs by Hsc70, playing a vital role in various diseases such as cancer and neurodegenerative diseases [1–3]. However, the detailed structural mechanism behind substrate recognition and the way Hsc70 binds to substrates is still not fully understood [4]. Here, we combined multiple computational approaches including AlphaFold 3 and molecular dynamics (MD) simulations to analyze the binding of 15 experimentally validated CMA substrates to human Hsc70. Detailed residue-level structural and thermodynamic analyses from 44μs of MD simulations revealed secondary binding sites in SBDα and SBDβ domain of Hsc70. The hydrophobic residues within the domains stabilized the substrates throughout the trajectory. Also, our study revealed preferences in conformational states of Hsc70 for binding with CMA substrates. The understanding gained from structural and thermodynamic studies of these binding interactions will support various therapeutic strategies and facilitate drug discovery.

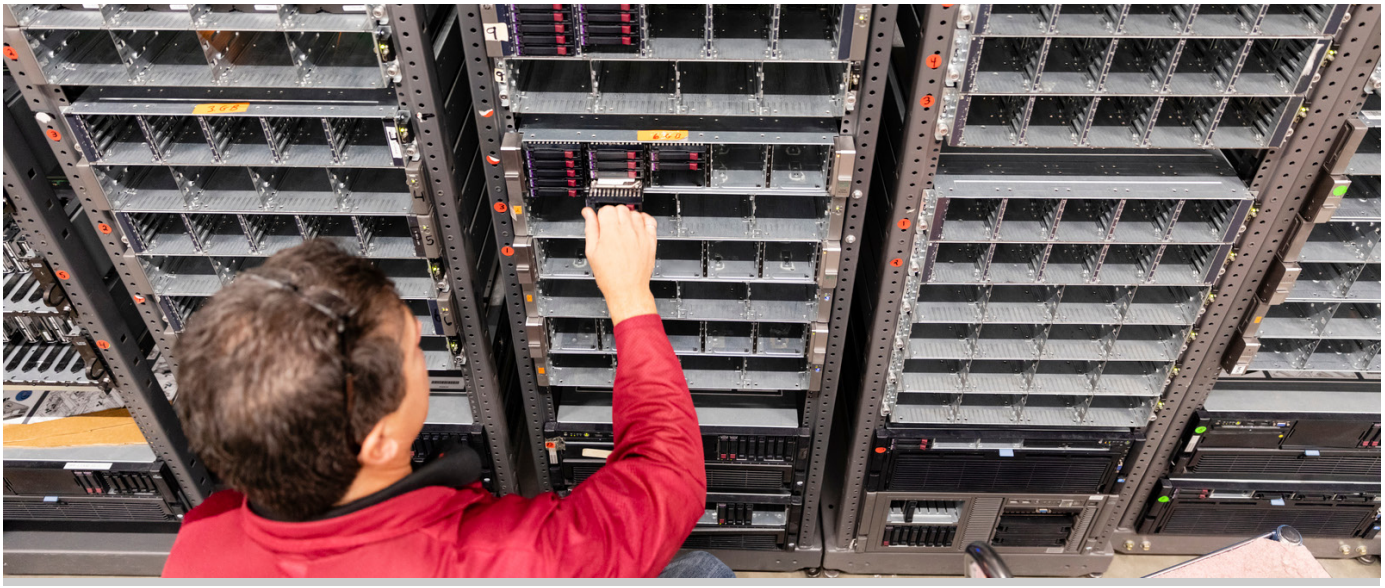


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HPE

Brochure

UNLEASH INNOVATION AND DISCOVERY IN THE AI ERA



High performance computing (HPC) is essential for today's most innovative scientific and industrial breakthroughs. When combined with AI and quantum technologies, HPC not only accelerates processes but also creates entirely new opportunities, fueling breakthroughs and setting the stage for the next era of innovation and global leadership.

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HPC systems that support AI enable researchers to virtually explore complex systems—from drug interactions to aerodynamic flows—long before creating physical prototypes. AI algorithms can continuously simulate, learn, and refine these models, offering significant savings in both time and cost. In industries such as finance, healthcare, and manufacturing, the combination of HPC and AI enables instant data analysis, predictive analytics, and smarter, faster decision-making, helping organizations stay ahead of the competition.

To gain a strategic advantage, accelerate breakthroughs, and achieve successful results in today's AI-driven world, organizations need supercomputing solutions built for HPC, AI, and various other workloads. The HPE high performance computing portfolio offers exactly that: world-class performance, continuous innovation, and exascale expertise to tackle your most demanding challenges—whether training large language models, running real-time analytics, or enabling next-generation discoveries.

Fast-track results with unmatched performance density

In today's relentless quest for breakthroughs, organizations face increasing pressure to outpace the competition and turn ambitious ideas into reality. The driving force behind this progress is HPC, which enables teams to make discoveries faster and smarter than ever before.

Imagine a future where massive workloads are viewed as opportunities instead of obstacles, and where training large language models and conducting high performance data analytics become routine rather than daunting tasks. Thanks to HPE's innovative HPC and AI platforms, that future is already here. Through HPE's advanced HPC and AI systems, organizations are achieving performance speeds once thought impossible.

The secret? HPE's unified architecture that combines the processing power of CPUs and GPUs, enabling seamless hybrid workflows. These industry-leading systems are designed specifically for the complexity of AI tasks and hybrid workloads, helping organizations overcome their biggest challenges.

The newest HPE Cray supercomputers further enhance this advantage, providing the highest compute density and the fastest I/O performance per rack available today.[1] This performance isn't just theoretical. HPE systems are regularly recognized among the TOP500 fastest supercomputers[2] and IO500 fastest storage solutions worldwide.[3] All this performance is delivered with industry-leading value, offering unmatched performance per dollar and per square foot or meter.

Unleash possibilities with breakthrough innovations

Organizations that use HPC systems constantly push the boundaries, requiring technologies that not only keep pace with progress but also drive it forward. This is where HPE Supercomputing excels. Unlike many competitors, HPE continues to invest in innovations that regularly advance the industry.

Our legacy of supercomputing leadership is demonstrated through numerous ongoing innovations.

- **An integrated platform:** HPE's unified platform effortlessly merges HPC and AI, letting you easily run both types of workloads side by side. Traditional physics-based modeling and simulations can interact directly with AI models, unleashing new possibilities. Our innovative architecture even supports access to quantum computing—letting you solve complex problems beyond the capabilities of classical systems.
- **Seamless integration and management:** HPE's software ecosystem offers full-stack support for HPC and AI, enabling smooth management of complex environments. Unified orchestration allows users to efficiently combine CPUs and GPUs, optimize workflows, and accelerate analytics. Deployment and scaling are streamlined, thanks to support for advanced storage and networking solutions.
- **Storage and networking leadership:** Data is expanding faster than ever, and HPE's scalable, high performance storage systems—featuring Lustre or DAOS—are built for the largest datasets and most demanding environments. Ultra-fast networking connects thousands of computers, processors, and storage devices to enable processing and analysis at unprecedented speeds.
- **Security expertise:** No breakthrough is possible without trust and security. HPE incorporates robust compliance, end-to-end encryption, and sovereign AI solutions, making HPE a preferred partner for governments and highly regulated industries worldwide.
- **Flexible deployment options:** Whether your workload runs on-premises, in the cloud, or spans both, HPE's unified management can provide a seamless experience. Flexible deployment options allow organizations to adapt their infrastructure to meet current needs and future goals.
- **Decades of pioneering research:** Over 60,000 patents and ongoing innovations from HPE Labs[4] give customers access to industry-leading technology.

Simplify complexity and speed outcomes with exascale expertise

As organizations face increasing data volumes and more complex challenges, the path to innovation can be hindered by slow communication, storage delays, and ongoing competition for system resources. The need for solutions that enable rapid deployment, maximize resource use, improve scaling, and deliver excellent energy efficiency is more important than ever.

HPE is uniquely capable of turning these challenges into opportunities. Supported by a global team of exascale experts, HPE collaborates closely with customers and partners to develop the world's most advanced computing systems. Through groundbreaking projects like El Capitan, Frontier, and Aurora, HPE has pushed the boundaries of HPC, setting standards in system design, seamless deployment, and application performance that others aim to replicate.

Yet, HPE's leadership extends beyond innovation. As the industry leader in designing, deploying, and supporting exascale systems featured on the esteemed TOP500 list, HPE offers unmatched expertise to every project on the path to exascale.

HPE is the only HPC system provider with practical experience in every stage of creating exascale-class systems, from initial design and rigorous testing to seamless deployment and continuous support. This extensive expertise covers system design, implementation, and optimization of application performance, offering customers proven HPC solutions.

Finally, 50 years of experience from Cray Supercomputer innovations provides HPE customers with energy-efficient, liquid-cooling technology. HPE delivers optimal thermal efficiency and dependable cooling performance on our HPC systems, enabling organizations to expand their HPC capabilities while decreasing energy use.

[1] Compared to Dell Integrated Rack IR7000 configured with Dell PowerEdge M7725 CPU servers or Dell PowerEdge XE8712 GPU servers with Dell PowerScale F710 All-Flash NAS storage.

[2] TOP500

[3] IO500

[4] HPE Labs was originally founded as HP Labs in 1966. It was renamed HPE Labs in 2015.

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CP2K ON 5TH GEN AMD EPYC™ PROCESSORS
QUANTUM CHEMISTRY

Powered by 5th Gen AMD EPYC™ Processors

October 2024

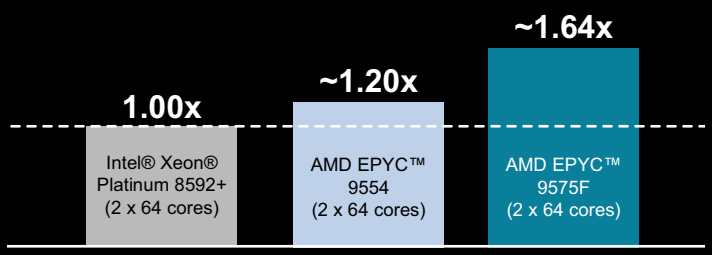
AT A GLANCE

A 2P system powered by 64-core 5th Gen AMD EPYC™ processors demonstrate outstanding performance uplifts versus a 2P system powered by 5th Gen Intel® Xeon® Platinum 8592+ processors running the CP2K H2O-dft-ls-NREP6 benchmark.

PERFORMANCE HIGHLIGHTS

A 2P 64-core 5th Gen AMD EPYC 9575F system (128 total cores) demonstrates an average ~1.64x uplift on the CP2K H2O-dft-ls-NREP6 workload vs. a 2P 64-core Intel® Xeon® Platinum 8592+ system (128 total cores). A 2P 64-core AMD EPYC 9554 system (128 total cores) outperforms the same Intel system by an average of ~1.20x on the same benchmark.

2P 4TH AND 5TH GEN AMD EPYC™ VS.
2P 5TH INTEL XEON PLATINUM 8592+



KEY TAKEAWAYS

64-core 4th and 5th AMD EPYC processors deliver solid performance uplifts running the CP2K H2O-dft-ls-NREP6 benchmark versus top of stack 5th Gen Intel Xeon Platinum 8592+ processors in dual-socket configurations. The 2P 4th Gen AMD EPYC 9554 system delivers a ~1.20x uplift, and the 2P 5th Gen AMD EPYC 9575F processor delivers a ~1.64x uplift using the same number of processor cores as the Intel Xeon Platinum 8592+ system.5th Gen AMD EPYC processors are available in 1P and 2P configurations and feature:

- Up to 128 "Zen 5" or 192 "Zen5c" cores.
- Up to 512 MB L3 cache in "Zen 5" AMD EPYC processors.
- Up to 4 links of Gen 3 Infinity Fabric™ at up to 32 Gbps.
- 12 memory channels that support up to 9 TB of DDR5-6000 memory.
- Support for PCIe® Gen 5 at up to 32 Gbps.
- AVX-512 instruction support for enhanced HPC and ML performance.
- AMD Infinity Guard technology to defend your data.[1]

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AMD EPYC 9005 PROCESSORS

5th Gen AMD EPYC processors are the newest generation of the powerful and efficient AMD EPYC processor family for servers that have set hundreds of world records for performance and efficiency. The AMD EPYC 9005 processor family is built on the breakthrough high performance, highly efficient "Zen 5" processor core architecture and advanced microprocessor process technologies to better meet the needs of the modern AI-enabled data center. The complete line of 5th Gen AMD EPYC processor offerings include a wide range of core counts (up to 192 cores and 384 threads per processor), max boost frequencies up to 5 GHz, generous L3 cache capacities, high energy efficiency, and competitive cost points. These cutting-edge technologies and features are all backed by the familiar x86 software compatibility that allows servers powered by AMD EPYC 9005 processors to readily support almost any business need.

SYSTEM CONFIGURATION

AMD SYSTEM CONFIGURATION		
CPUs	2 x AMD EPYC™ 9554	2 x AMD EPYC™ 9575F
Frequency: Base | Boost[2]	3.1 GHz | 3.75 GHz	3.3 GHz | 5.0 GHz
Cores	64 cores/socket (128 threads)	64 cores/socket (128 threads)
L3 Cache	256 MB per CPU	256 MB per CPU
Memory	1.5 TB (24 x 64 GB DDR5-4800)	1.5 TB (24 x 64 GB DDR5-6000)
Storage	SAMSUNG MZQL21T9HCJR-00A07	SAMSUNG MZWLO3T8HCLS-00A07
BIOS Version	RTI1009C	RVOT1000C
BIOS Settings	SMT=Off, NPS=4, Determinism=Power	
OS	RHEL 9.4 (kernel 5.14.0- 427.16.1.el9_4.x86_64)	
OS Settings	amd_iommu=on, iommu=pt, mitigations=off	

Table 1: AMD system configurations

INTEL SYSTEM CONFIGURATION	
CPUs	2 x Intel® Xeon® PLATINUM 8592+
Frequency: Base | Boost	1.9 GHz | 3.9 GHz
Cores	64 cores/socket (128 threads)
L3 Cache	320 MB per CPU
Memory	1.0 TB (16 x 64 GB DDR5-5600)
Storage	KIOXIA KCMYXRUG3T84
BIOS Version	ESE122V-3.10
BIOS Settings	Hyperthreading=Off, High Performance Mode
OS	RHEL 9.4 (kernel 5.14.0-427.16.1.el9_4.x86_64)
OS Settings	processor.max_cstate=1, intel_idle.max_cstate=0, iommu=pt, mitigations=off

Table 2: Intel system configurations

TEST METHODOLOGY

CP2K provides a standard set of benchmarks that evaluate the performance of different platforms running CP2K applications. These benchmark cases represent typical usage and cover a range of sizes. The uplift is calculated as the ratio of the systems under test (*sut*) to the reference systems (*ref*) based on an average of three test runs per benchmark. In this Performance Brief, the Intel Xeon Platinum 8592+ processors were the *ref* system, and the 4th and 5th Gen AMD EPYC processors were the *sut* for the competitive uplift. The results presented in this Performance Brief are the average per-processor uplifts running the H2O-dft-ls-NREP6 benchmark. The systems tested were configured as shown in Tables 1 and 2, above.

FOR ADDITIONAL INFORMATION

Please see the following additional resources for more information about 5th Gen AMD EPYC features, architecture, and available models:

- AMD EPYC™ Processors
- AMD Documentation Hub

REFERENCES

1. AMD Infinity Guard features vary by EPYC™ Processor generations and/or series. Infinity Guard security features must be enabled by server OEMs and/or Cloud Service Providers to operate. Check with your OEM or provider to confirm support of these features. Learn more about Infinity Guard at http://www.amd.com/en/products/processors/server/epyc/infinity-guard.html. GD-183A
2. Maximum boost for AMD EPYC processors is the maximum frequency achievable by any single core on the processor under normal operating conditions for server systems. EPYC-18

AUTHORS
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RELATED LINKS

- CP2K*
- AMD EPYC™ Processors
- AMD Documentation Hub

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AMD EPYC 9004 FOR QUANTUM CHEMISTRY

4th Gen AMD EPYC CPUs deliver excellent performance by taking advantage of fast CPU frequencies, low latency memory, and a unified cache structure. Scientists and researchers can use AMD EPYC processors to apply the principles of quantum mechanics to study atomic and molecular behavior with ground-breaking high-performance computing and robust security features to deliver excellent results.

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AMD EPYC 9005 Series Processors support up to:

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- Up to 512 MB of L3 cache per CPU
- 32 MB of L3 cache per CCD
- 9 TB of DDR5-6000 memory
- Up to 128 (1P) or 160 (2P) PCIe® Gen 5 lanes

Infinity Guard security features[1]

- Secure Boot
- Encrypted memory with SME

CP2K

CP2K is a quantum chemistry and solid state physics software package that can perform atomistic simulations of solid state, liquid, molecular, periodic, material, crystal, and biological systems. CP2K provides a general framework for different modeling methods such as DFT using the mixed Gaussian and plane waves approaches GPW and GAPW.

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QUANTUM ESPRESSO ON 5TH GEN AMD EPYC™ PROCESSORS
MOLECULAR DYNAMICS SIMULATIONS

Powered by 5th Gen AMD EPYC™ Processors

October 2024

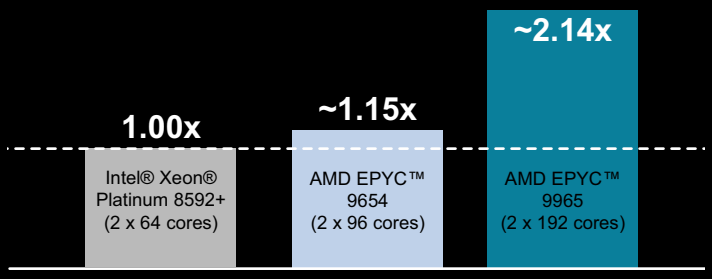
AT A GLANCE

A 2P system powered by 192-core 5th Gen AMD EPYC™ processors demonstrate outstanding performance uplifts versus a 2P system powered by 5th Gen Intel® Xeon® Platinum 8592+ processors running select Quantum ESPRESSO benchmarks.

PERFORMANCE HIGHLIGHTS

A 2P 192-core 5th Gen AMD EPYC 9965 system (384 total cores) demonstrates a composite average ~2.14x uplift on select Quantum ESPRESSO workloads vs. a 2P 64-core Intel® Xeon® Platinum 8592+ system (128 total cores). A 2P 96-core AMD EPYC 9654 system (192 total cores) outperforms the same Intel system by a composite average of ~1.15x. Please see Page 2 for detailed per-benchmark results.

2P 4TH AND 5TH GEN AMD EPYC™ VS.
2P 5TH INTEL XEON PLATINUM 8592+



KEY TAKEAWAYS

A 2P system powered by 192-core 5th Gen AMD EPYC 9965 processors (384 total cores) demonstrates a maximum uplift of ~2.40x versus a 2P system powered by a 64-core 5th Gen Intel Xeon 8592+ processors (128 total cores) running the Quantum ESPRESSO qe-7.0_Ausurf workload. A 2P system powered by 96-core 4th Gen AMD EPYC 9654 processors (192 total cores) demonstrates a maximum uplift of ~1.16x running the Quantum ESPRESSO qe-7.0_Ta205 workload versus the same Intel system. Detailed per-benchmark results appear on Page 2.

5th Gen AMD EPYC processors are available in 1P and 2P configurations and feature:

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- Up to 512 MB L3 cache in "Zen 5" AMD EPYC processors.
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- AVX-512 instruction support for enhanced HPC and ML performance.
- AMD Infinity Guard technology to defend your data.[1]

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DETAILED RESULTS

This section presents the detailed per-benchmark results for the systems described in Tables 1 and 2, below. Please see the chart at the top of Page 1 for the composite average performance results for both AMD EPYC processors.

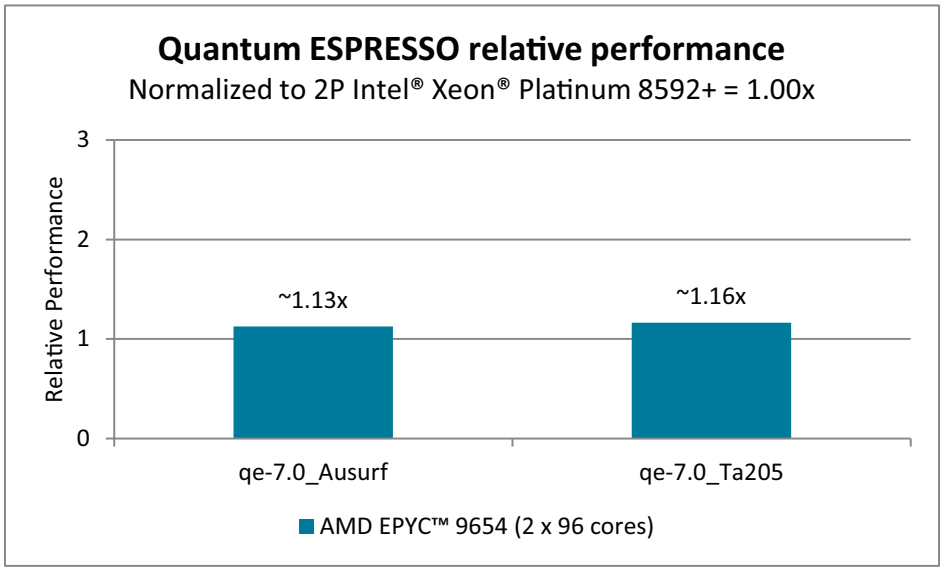


Figure 1: Relative 2P 4th Gen AMD EPYC 9654 per-benchmark Quantum ESPRESSO results vs. 2P 5th Gen Intel Xeon 8592+

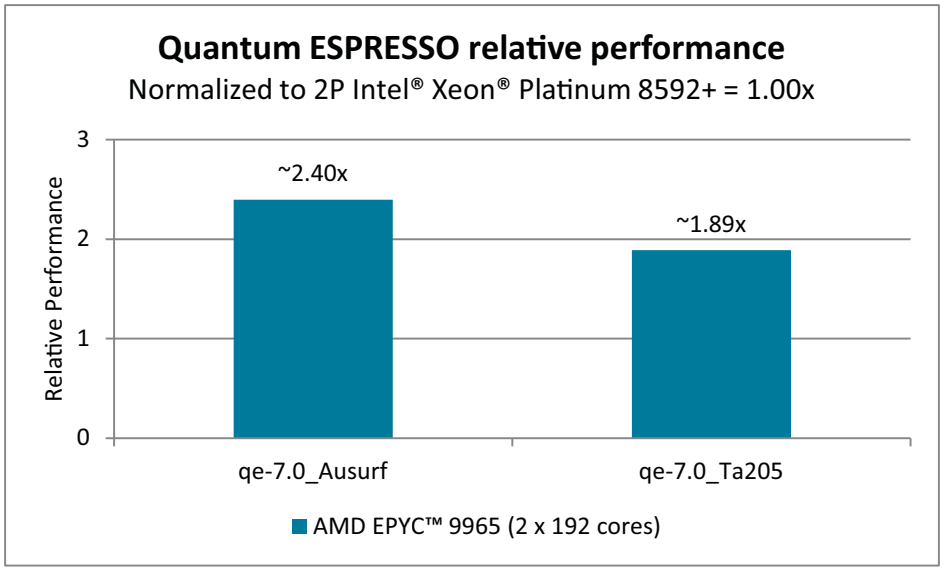


Figure 2: Relative 2P 5th Gen AMD EPYC 9965 per-benchmark Quantum ESPRESSO results vs. 2P 5th Gen Intel Xeon 8592+

AMD EPYC 9005 PROCESSORS

5th Gen AMD EPYC processors are the newest generation of the powerful and efficient AMD EPYC processor family for servers that have set hundreds of world records for performance and efficiency. The AMD EPYC 9005 processor family is built on the breakthrough high performance, highly efficient "Zen 5" processor core architecture and advanced microprocessor process technologies to better meet the needs of the modern AI-enabled data center. The complete line of 5th Gen AMD EPYC processor offerings include a wide range of core counts (up to 192 cores and 384 threads per processor), max boost frequencies up to 5 GHz[2], generous L3 cache capacities, high energy efficiency, and competitive cost points. These cutting-edge technologies and features are all backed by the familiar x86 software compatibility that allows servers powered by AMD EPYC 9005 processors to readily support almost any business need.

SYSTEM CONFIGURATION

AMD SYSTEM CONFIGURATION		
CPUs	2 x AMD EPYC™ 9654	2 x AMD EPYC™ 9965
Frequency: Base | Boost[2]	2.4 GHz | 3.7 GHz	2.25 GHz | 3.7 GHz
Cores	96 cores/socket (192 threads)	192 cores/socket (256 threads)
L3 Cache	256 MB per CPU	384 MB per CPU
Memory	1.5 TB (24 x 64 GB DDR5-4800)	1.5 TB (24 x 64 GB DDR5-6000)
Storage	SAMSUNG MZQL21T9HCJR-00A07	SAMSUNG MZWLO3T8HCLS-00A07
BIOS Version	RTI1009C	RVOT1000C
BIOS Settings	SMT=Off, NPS=4, Determinism=Power	
OS	RHEL 9.4 (kernel 5.14.0- 427.16.1.el9_4.x86_64)	
OS Settings	amd_iommu=on, iommu=pt, mitigations=off	

Table 1: AMD system configurations

INTEL SYSTEM CONFIGURATION	
CPUs	2 x Intel® Xeon® PLATINUM 8592+
Frequency: Base | Boost	1.9 GHz | 3.9 GHz
Cores	64 cores/socket (128 threads)
L3 Cache	320 MB per CPU
Memory	1.0 TB (16 x 64 GB DDR5-5600)
Storage	KIOXIA KCMYXRUG3T84
BIOS Version	ESE122V-3.10
BIOS Settings	Hyperthreading=Off, High Performance Mode
OS	RHEL 9.4 (kernel 5.14.0-427.16.1.el9_4.x86_64)
OS Settings	processor.max_cstate=1, intel_idle.max_cstate=0, iommu=pt, mitigations=off

Table 2: Intel system configurations

TEST METHODOLOGY

Quantum ESPRESSO provides a standard set of benchmarks that evaluate the performance of different platforms running Quantum ESPRESSO applications. These benchmark cases represent typical usage and cover a range of sizes. The uplift is calculated as the ratio of the systems under test (*sut*) to the reference systems (*ref*) based on an average of three test runs per benchmark. In this Performance Brief, the Intel Xeon Platinum 8592+ processor is the *ref* system, and 4th and 5th Gen AMD EPYC processors are the *sut*. The total amount of variability between individual runs was <1%. The results presented in this Performance Brief are the Quantum ESPRESSO benchmarks shown in Figures 1 and, 2above. The systems tested were configured as shown in Tables 1 and 2, above.

FOR ADDITIONAL INFORMATION

Please see the following additional resources for more information about 5th Gen AMD EPYC features, architecture, and available models:

- AMD EPYC™ Processors
- AMD Documentation Hub

REFERENCES

1. AMD Infinity Guard features vary by EPYC™ Processor generations and/or series. Infinity Guard security features must be enabled by server OEMs and/or Cloud Service Providers to operate. Check with your OEM or provider to confirm support of these features. Learn more about Infinity Guard at http://www.amd.com/en/products/processors/server/epyc/infinity-guard.html. GD-183A
2. Maximum boost for AMD EPYC processors is the maximum frequency achievable by any single core on the processor under normal operating conditions for server systems. EPYC-18

AUTHORS

Alvaro Fernandez, Jaber JavanshirHasbestan, Wilmer FinolInciarte, and Michael Senizaiz

RELATED LINKS

- Quantum ESPRESSO*
- AMD EPYC™ Processors
- AMD Documentation Hub

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AMD EPYC 9005 FOR MOLECULAR DYNAMICS

5th Gen AMD EPYC CPUs deliver excellent performance by taking advantage of fast CPU frequencies, low latency memory, and a unified cache structure. Biologists and geneticists can use AMD EPYC processors to perform complex DNA sequencing and other molecular dynamics simulations with ground-breaking high-performance computing and robust security features to deliver excellent results.

"ZEN 5" CORE & SECURITY FEATURES

AMD EPYC 9005 Series Processors support up to:

- 192 physical cores, 384 threads
- Up to 512 MB of L3 cache per CPU
- 32 MB of L3 cache per CCD
- 9 TB of DDR5-6000 memory
- Up to 128 (1P) or 160 (2P) PCIe® Gen 5 lanes

Infinity Guard security features[1]

- Secure Boot
- Encrypted memory with SME

QUANTUM ESPRESSO

Quantum ESPRESSO is a suite of open-source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials. The Quantum ESPRESSO distribution consists of a "historical" core set of components, and a set of plug-ins that perform more advanced tasks, plus a number of third-party packages designed to be inter-operable with the core components.

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A brief profile of Lenovo



Lenovo has a history of over 21 years of technology innovation in areas that include advanced server technology, datacenter energy efficiency and management. Lenovo's technology leadership is widely recognized in the industry.

1. Lenovo offers complete Portfolio from mobile device, PCs, edge to Data Centre
2. Fortune Global 500 (#196) company with over US$69 billion annual revenue
3. #1 in ITIC's x86 server reliability for a 11th year in a row)
4. HPCWire Best HPC Server Product or Technology
5. The Lenovo ThinkSystem servers currently hold 650 world record in Workload Performance
6. Ranked # 1 in Top 500 list released in Nov 2025 with 141 entries.
7. Direct Warm Water cooled Cluster Installation in Indat at LPSC Trivandrum and many in WW.



We have a proven track record: Datacenter management and redundancy is increasingly moving to the software layer. IT Directors need the hardware platform to be standardized to give them the flexibility they need to transition their datacenter into a software-defined infrastructure. Server manufacturers who have the best products combined with lowest costs will win. And that is exactly who Lenovo is. A decade ago, the PC industry went through a similar wave of reform. All of the lessons that we absorbed in our journey to becoming the world's #1 PC manufacturer are now applied in our mission to become the world's #1 server manufacturer.

Lenovo High Performance Computing

Lenovo HPC Team

The High-Performance Computing business that IBM created and cultivated in ThinkSystem was of particular interest to Lenovo. Lenovo understands that in order to effectively compete in the HPC space, we must invest not only in products and a robust portfolio but also in critical skills.



During the divestiture of System X, Lenovo worked closely with IBM to ensure that the critical skills in areas such as thermal design, performance optimization, Systems Management, Storage, and high-speed fabric. were retained and brought into the Lenovo family. We now continue our drive for excellence in HPC thanks to the deep HPC skillsets we have across the spectrum of sales, technical sales, development, service and support.

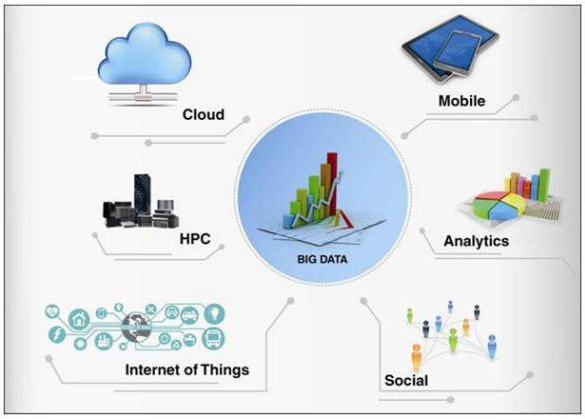
The Lenovo HPC team is singularly focused on developing and architecting solutions that are optimized on x86 platforms. At Lenovo, this team is truly open and committed to providing solutions that are designed to benefit our customers. Lenovo HPC has no other commitments other than to focus on delivering value to the HPC community. This approach is novel in the industry in that our partnerships are formed solely with the customer rather than being driven by other parts of the business or OEM relationships. This change allows the Lenovo HPC team to become familiar with all technology in the industry and be able to recommend the best-of-breed solution that they can stand behind. Our broad partnerships with industry leaders such as Intel, Mellanox, Qlogic, DDN, EMC, NVIDIA and others has strengthened as a result.

Lenovo is deeply committed to innovation in all areas of its business from mobile to PCs to high end computing systems. For example, Lenovo's Research and Technology (R&T) group is working on innovative ways to accelerate computing in analytics by using accelerators. Each team in the R&T group is led by a Master Inventor in areas such as GPGPU acceleration, Mobile Technologies, Cloud, and Datacenter Energy Efficiency to name a few. Lenovo adopted specialized criteria when awarding someone the title of Master Inventor as a significant portion of the technical leadership culture.

Lenovo Center of Competency

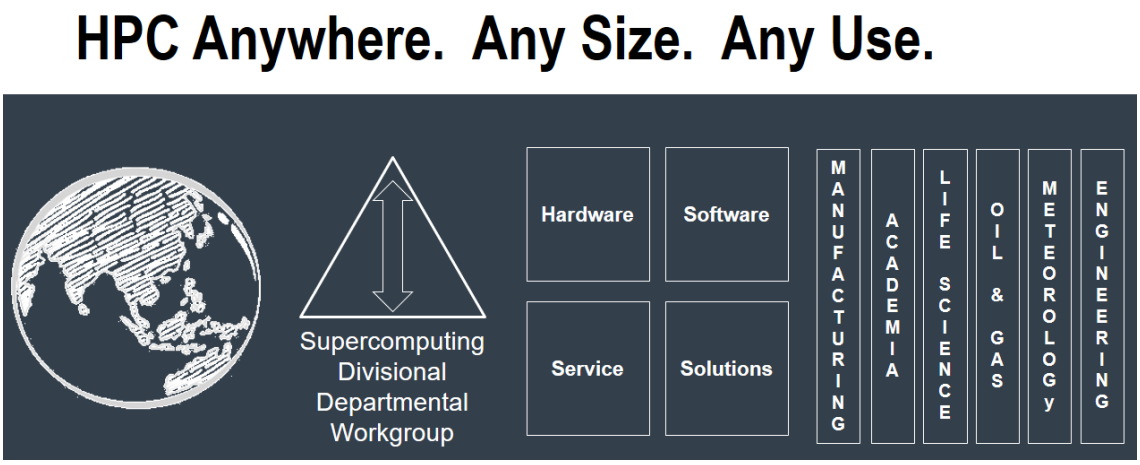
The Lenovo HPC Center of Competency is a sales engineering organization with the role of delivering excellence in HPC solution design, benchmarking, deployment, and customer experience. There are nearly 30 HPC Center of Competency professionals worldwide.

The HPC Center of competency is organized into 6 geographies worldwide, with teams in North America, Europe, Greater China, the Middle East, and Asia Pacific. Each geography has a local leader reporting up to a single worldwide leader, all with a consistent mission and purpose.



In addition to delivering excellence HPC solution design as architects, our segment leaders have deep HPC expertise in specific market segments, including higher education & government, CAE/Auto/Aero, Weather/Climate, Financial, Pharmaceutical and Bio Science, and Oil and Gas.

The HPC Center of Competency operates the Lenovo HPC Innovation Center, which is a technology leadership research and development center for advancing HPC. Its mission is focused on support of the Lenovo HPC business, our partners, and our clients, including collaboration with industry leaders and visionary client partners. The flagship location is based in Budapest, Hungary and provides global benchmarking, proof of concept, and solution demonstration capabilities globally.

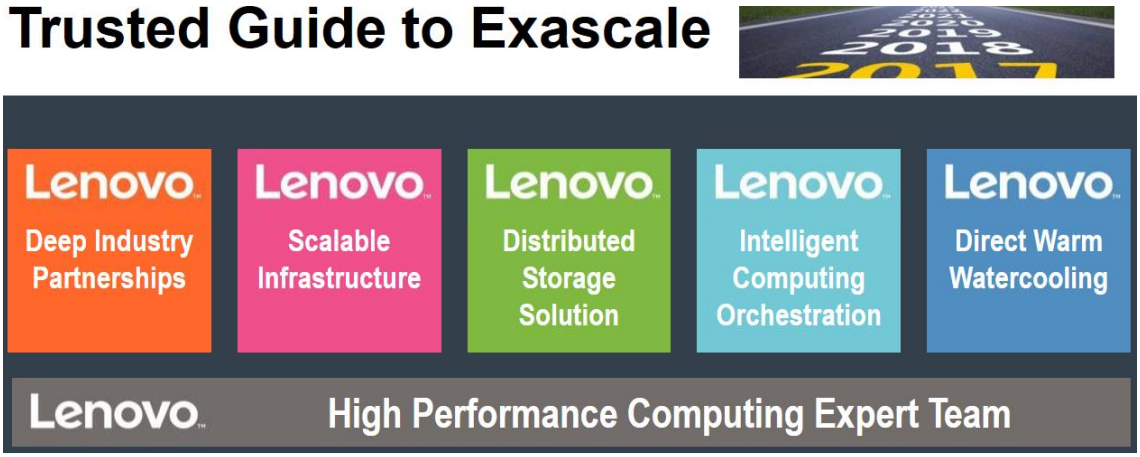


Lenovo HPC Research & Development

Lenovo continues commitment to R&D investment to establish the Lenovo HPC Innovation Center which was announced in 2015. This Innovation Center offers a permanent R&D and application benchmarking site as well as a new ecosystem of partners that will collaborate on projects to bring the commercial benefits of HPC to a broader spectrum of clients and workloads. Located in Budapest Hungary, the center marks Lenovo's commitment to enterprise computing and ambitions to become the number one Open Systems vendor in the market.

Working closely with Intel, the center offers the latest Intel Xeon scalable processor with both Mellanox InfiniBand and Intel Omni-Path interconnect fabrics leveraging Lenovo's Think System as the base compute platform. It will leverage the deep knowledge and specific skills of several specialized client partners from across Europe that will collaborate to further expand capabilities and advance localized research.





In addition to the Hungary HPC Innovation Center, Lenovo has 7 design centers worldwide as well as dedicated HPC Application teams.

Within the design centers, the teams are focused on innovations in areas such as compute, storage and high-speed networking, and efficiencies in power, cooling and mechanical engineering as well as firmware and scalable management (located in the Morrisville, NC development center, India Bangalore).

Lenovo HPC History and Roadmaps

There is a misperception about Lenovo that we are new to HPC. It's important to note that the Lenovo ThinkSystem business has a successful 20-year history in High Performance Computing. This history has deep roots in innovation. System X was the first brand in history to deliver sustained petaflop performance on LINPACK using only x86 cores. Blade server technology was developed and launched by the System X brand and that same technology was used to power the first petaflop system.

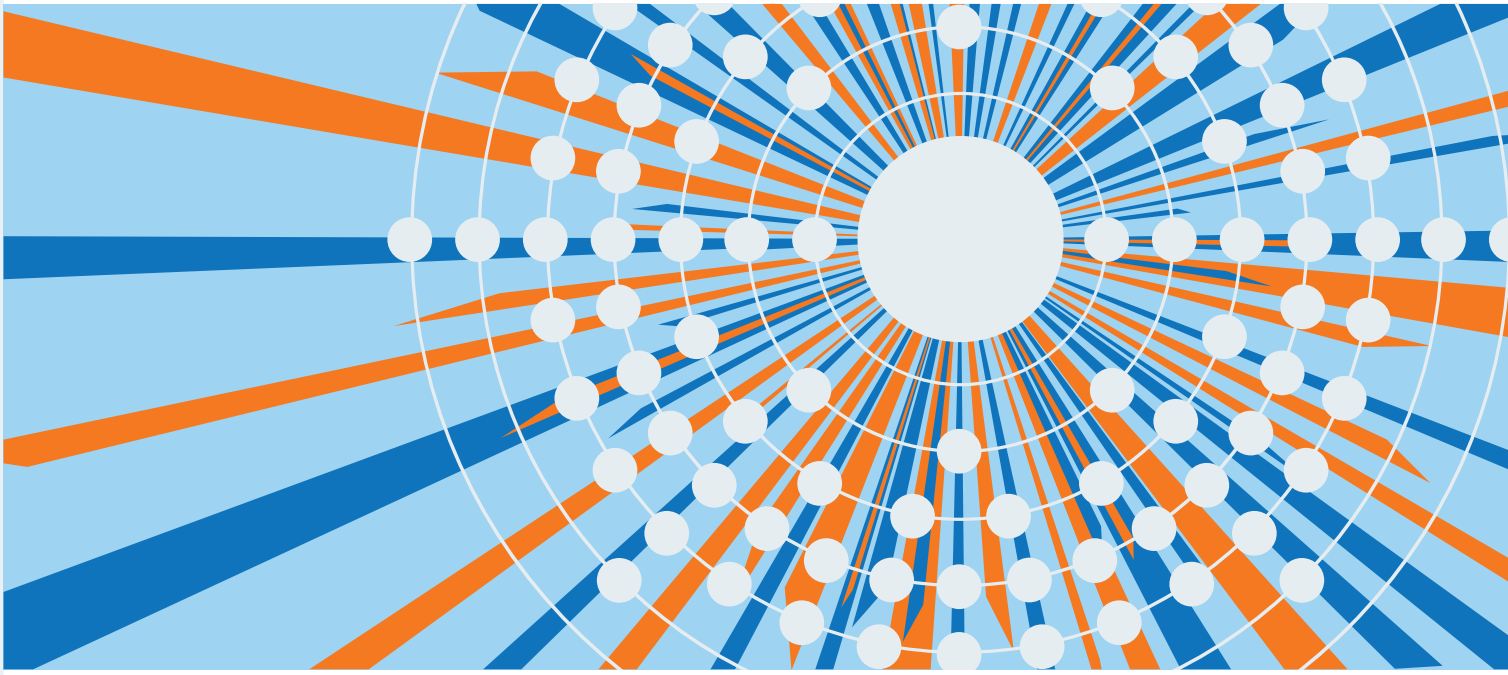
Recognizing the need for denser, power efficient systems, System X developed iDataPlex which ushered in the era of dense computing. NeXtScale improved on the iDataPlex design and delivered dense computing systems in industry standard racks. Lenovo is committed to driving dense, HPC-friendly solutions in line with Intel's technology roadmap into the 2010's and beyond and will continue to be an innovator and key player in this space with ThinkSystems.

We will continue to innovate in HPC through adoption of best-of-breed technologies into our platforms as well as designing novel approaches to computing such as liquid cooling, and dense, high-performance, reliable storage solutions. The following diagram gives a brief outline of our commitment to HPC which we intend to drive forward as Lenovo.

As the HPC industry continues to look for faster, less expensive ways to drive computing innovation, Lenovo intends to be engaged with the technical community in pioneering and driving innovation. Our current roadmaps expand on existing trends and look to leverage all areas of innovation such as IoT, hyperscale and enterprise computing to drive our HPC roadmaps.

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Alfred Nobel (1833–1896)

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This illustration was created by one of the talented team of designers at Springer Nature.

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Drive Innovation and Expedite Discovery with our HPC Solutions

- Scalable Clusters
- Zero-Hassle Deployments
- Expertise in hybrid architectures with CPU-GPU integration
- Tailor made Performance
- Customized HPC Solutions for Different Industry
- Smart Operations

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- Improved speed & greater capacity
- Quick setup & smooth integration
- Advanced simulations in low cost
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- Significant expansion and growth
- Quicker deployment of AI Models

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