



ICMS 2026

**7th International Conference
on Molecular Simulation**

Book of Abstracts



4–8 October 2026

**J. N. Tata Auditorium
Indian Institute of Science
Bengaluru, India**

About the conference

The 7th International Conference on Molecular Simulation brings together researchers working on the theory, methods and applications of molecular simulation. ICMS 2026 takes place from 4 to 8 October 2026 at the J. N. Tata Auditorium, Indian Institute of Science, Bengaluru.

This book presents the scientific programme and abstracts for plenary, keynote, invited and contributed talks. The abstracts are arranged in programme order, by date, session and hall.

Scientific themes

- Biological Systems and Medicine
- Catalysis and Surface Science
- Computational Material Sciences
- Machine Learning and AI, and Molecular Modeling
- Theory and Methodology
- Polymers and Soft Matter
- Energy
- Materials and Biological Systems

Using this book

In the compiled PDF, select a speaker name in the scientific programme to open that contribution. The contents link to each conference day, and PDF bookmarks provide another route to dates, sessions and individual abstracts. Each abstract begins on a new page.

The scientific programme appears as a separate section near the beginning of the book. Session times, venues and talk categories follow that programme.

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Scientific Program Schedule

The 7th International Conference on Molecular Simulation (ICMS 2026)

4-8 October 2026 | J. N. Tata Auditorium, Indian Institute of Science, Bengaluru

- **Talk durations:** Plenary 40 min; **Keynote 30 min; Invited 20 min; Contributed 15 min**
- **Number of Talks:** 6 Plenary; **22 Keynote; 79 Invited; 60 Contributed**
- **Parallel themes:**
 - Biological Systems and Medicine (6 sessions)
 - Catalysis and Surface Science (3 sessions)
 - Computational Material Sciences (3 sessions)
 - Machine Learning and AI, and Molecular Modeling (6 sessions)
 - Theory and Methodology (3 sessions)
 - Polymers and Soft Matter (4 sessions)
 - Energy (1 session)
 - Materials and Biological Systems (1 session).

Sunday, 4 October 2026

Time	J. N. Tata Auditorium
16:00-19:00	REGISTRATION AND KIT DISTRIBUTION
17:00-19:00	WELCOME RECEPTION

Monday, 5 October 2026

Time	Main Auditorium	Hall A	Hall B	Hall C
08:00-09:00	REGISTRATION			
09:00-09:30	INAUGURATION / WELCOME ADDRESS – Main Auditorium			
09:30-10:10	PLENARY LECTURE I – Main Auditorium J. Ilja. Siepmann, University of Minnesota, Minneapolis, USA (Chair: Ganapathy Ayappa)			
10:10-10:30	Tea break			
10:30-12:30	Parallel Session I Biological Systems and Medicine Chair: Nobuyuki Matubayasi Keynote Talk: Florence Tama Invited Talk: Jun Soo Kim Invited Talk: Ricky Nellas Contributed Talk: Arvinpreet Kaur Contributed Talk: Stefan Hervø-Hansen Contributed Talk: Sudipto Muhuri	Parallel Session I Computational Material Sciences Chair: Jayant K Singh Keynote Talk: Shiang-Tai Lin Invited Talk: Bong June Sung Invited Talk: Priya Johari Contributed Talk: Unity Ekugbe Oluwaiye Contributed Talk: Sahane Nisha Contributed Talk: Chaitanya Jitendra Shah	Parallel Session I ML/AI and Molecular Modeling Chair: Balasubramanian Sundaram Keynote Talk: Jhih-Wei Chu Invited Talk: Kaito Takahashi Invited Talk: Anirban Mondal Contributed Talk: Sridip Parui Contributed Talk: Karan Deep Sharma	Parallel Session I Catalysis and Surface Science Chair: Lisa Roy Keynote Talk: Hyungjun Kim Invited Talk: Ateeque Malani Invited Talk: Anil Boda Contributed Talk: Minho M. Kim Contributed Talk: Naiwrit Karmodak Contributed Talk: Jaewoo Jeong
12:30-14:00	LUNCH			
14:00-14:40	PLENARY LECTURE II – Main Auditorium Amalendu Chandra, Indian Institute of Technology Kanpur, India (Chair: Hyungjun Kim)			
14:40-15:00	TEA BREAK			
15:00-17:00	Parallel Session II Biological Systems and Medicine Chair: Manoj Varma Keynote Talk: Garima Jindal Invited Talk: Yuan-Chung Invited Talk: Sudip Das Invited Talk: Abhishek Sirohiwal Contributed Talk: Aditya Kumar Contributed Talk: Sangeetha Balasubramanian	Parallel Session II Theory and Methodology Chair: Amalendu Chandra Keynote Talk: Nisanth N Nair Invited Talk: Shinji Saito Invited Talk: Phani Motamarri Invited Talk: Susmita Roy Contributed Talk: Ryoma Sasaki Contributed Talk: Praveen Kumar Bommineni	Parallel Session II Polymers and Soft Matter Chair: Neelanjana Sengupta Keynote Talk: Nobuyuki Matubayasi Invited Talk: Takahiro Murashima Invited Talk: Debayan Chakraborty Invited Talk: BL Bhargava Contributed Talk: Takahiro Koishi Contributed Talk: Shubham Kumar	Parallel Session II Energy Chair: Hemant Kumar Invited Talk: Abhishek Aggarwal Invited Talk: Lukman Hakim Invited Talk: Yoshitaka Tateyama Invited Talk: Arun Venkatnathan Contributed Talk: Dhileep Nagi Reddy Thummuru Contributed Talk: Srikanth Divi
17:00-19:00	POSTER SESSION I + High Tea			

Tuesday, 6 October 2026

Time	Main Auditorium	Hall A	Hall B	Hall C
09:30-10:10	PLENARY LECTURE III – Main Auditorium Sang Soo Han, KIST, South Korea (Chair: Prabal Maiti)			
10:10-10:30	TEA BREAK			
10:30-12:30	Parallel Session III Biological Systems and Medicine Chair: Anand Srivastava Keynote Talk: Durba Sengupta Invited Talk: Min-Yeh Tsai Invited Talk: Ai Niitsu Contributed Talk: Aswin Vinod M Chockalingam Contributed Talk: Debabrata Pramanik	Parallel Session III Computational Material Sciences Chair: Subir Das Keynote Talk: Ananya Debnath Invited Talk: Vladimir Stegailov Contributed Talk: Swagata Pahari Contributed Talk: Sachin Aditya Ramesh Contributed Talk: Meena Devi J Contributed Talk: Binu Varghese	Parallel Session III ML/AI and Molecular Modeling Chair: Jagannath Mondal Keynote Talk: Jer-Lai Kuo Invited Talk: Jack Evans Invited Talk: Kartik Sau Invited Talk: Musharaf Ali Sheikh Contributed Talk: Jihoo Kim Contributed Talk: Swathi Srinivasan	Parallel Session III Theory and Methodology Chair: Florence Tama Keynote Talk: Alan Mark Invited Talk: Tod Pascal Invited Talk: Shinichi Miura Invited Talk: Sudeep Punnathanam Contributed Talk: Suvadip Das Contributed Talk: Manas Sharma
12:30-14:00	Lunch			
14:00-14:40	PLENARY LECTURE IV – Main Auditorium Yuji Sugita, RIKEN, Japan (Chair: Ananth Govind Rajan)			
14:40-15:00	TEA BREAK			
15:00-17:00	Parallel Session IV Biological Systems and Medicine Chair: R. Venkatramani Keynote Talk: Ganapathy Ayappa Invited Talk: Toshifumi Mori Invited Talk: Padmesh Anjukandi Invited Talk: Arnab Mukherjee Contributed Talk: Milan Kumar Hazra Contributed Talk: Sanjoy Paul	Parallel Session IV ML/AI and Molecular Modeling Chair: Jer-Lai Kuo Keynote Talk: Yousung Jung Invited Talk: Sungwoo Kang Invited Talk: Balasubramanian Sundaram Invited Talk: Dibyajyoti Ghosh Contributed Talk: Dr. Ravi Kumar Reddy Addula	Parallel Session IV Polymers and Soft Matter Chair: Bong June Sung Keynote Talk: Takeshi Kawasaki Invited Talk: Prateek Jha Invited Talk: YongJoo Kim Invited Talk: Yves Lansac Invited Talk: Kazushi Fujimoto	Parallel Session IV Catalysis and Surface Science Chair: Swapan Pati Invited Talk: Tej Choksi Invited Talk: Nitish Govindarajan Invited Talk: Akira Nakayama Contributed Talk: Debdip Bhandary Contributed Talk: Aravindhan Ramachandran
17:00-19:00	POSTER SESSION II + High Tea (18:00-18:45: International Advisory Committee Meeting)			
19:00-21:30	CONFERENCE BANQUET			

Wednesday, 7 October 2026

Time	Main Auditorium	Hall A	Hall B	Hall C
09:30-10:10	PLENARY LECTURE V – Main Auditorium Satyavani Vemparala, The Institute of Mathematical Sciences, Chennai, India (Chair: Durba Sengupta)			
10:10-10:30	TEA BREAK			
10:30-12:30	Parallel Session V Biological Systems and Medicine Chair: Arnab Mukherjee Keynote Talk: Wataru Shinoda Invited Talk: Shachi Gosavi Invited Talk: Srabani Taraphder Invited Talk: Himanshu Joshi Contributed Talk: Subbarao Kanchi Contributed Talk: Abhinava Chatterjee	Parallel Session V ML/AI and Molecular Modeling Chair: Musharaf Ali Sheikh Keynote Talk: Guan Hua Chen Invited Talk: Jagannath Mondal Invited Talk: Shelaka Gupta Invited Talk: Biman Jana Contributed Talk: Kumari Soniya Contributed Talk: Yogendra Kumar	Parallel Session V Polymers and Soft Matter Chair: Prasenjit Sen Keynote Talk: Yun Hee Jang Invited Talk: Neelanjana Sengupta Invited Talk: Kun-Han Lin Invited Talk: Shibananda Das Contributed Talk: Prateek Chowdhury Contributed Talk: Vrinda Garg	Parallel Session V Catalysis and Surface Science Chair: Padma Kumar Padmanabhan Keynote Talk: Nikos Doltsinis Invited Talk: Ananth Govind Rajan Invited Talk: Lisa Roy Contributed Talk: Dr. Aritri Biswas Contributed Talk: Jijo Johnson
12:30-14:00	LUNCH			
14:00-14:40	PLENARY LECTURE VI – Main Auditorium Roland Netz, FU Berlin, Germany (Chair: Sudeep Punnathanam)			
14:40-15:00	TEA BREAK			
15:00-17:00	Parallel Session VI Polymers and Soft Matter Chair: Prateek Jha Invited Talk: Sutapa Roy Invited Talk: Sanjay Kumar Invited Talk: Jure Dobnikar Invited Talk: Nirmalya Bachhar Invited Talk: Kang Kim Contributed Talk: Jayeeta Chattopadhyay	Parallel Session VI ML/AI and Molecular Modeling Chair: Ananya Debnath Keynote Talk: Supawadee Namuangruk Invited Talk: Hemant Kumar Invited Talk: Prasenjit Sen Invited Talk: Sai Gautam Invited Talk: Gopalakrishnan Contributed Talk: Mithun Biswas Contributed Talk: Varad Daoo	Parallel Session VI Theory and Methodology Chair: Ateeque Malani Invited Talk: Debashree Chakraborty Invited Talk: Susumu Okazaki Invited Talk: Santosh Mogurampelly Invited Talk: Kento Kasahara Invited Talk: Ravindra Venkatramani Contributed Talk: Anil Kumar Sahoo	Parallel Session VI Industry / Special Session Chair: Ananth Govind Rajan Invited Talk: Somananda Sanyal, Wiley Invited Talk: Ritwik Kavathekar, Biovia, Dassault Systemes Invited Talk: Ashutosh, Micropoint Computers Pvt. Ltd. Invited Talk: National Program on Technology Enhanced Learning (NPTEL)
17:00-19:00	POSTER SESSION III + High Tea			

Thursday, 8 October 2026

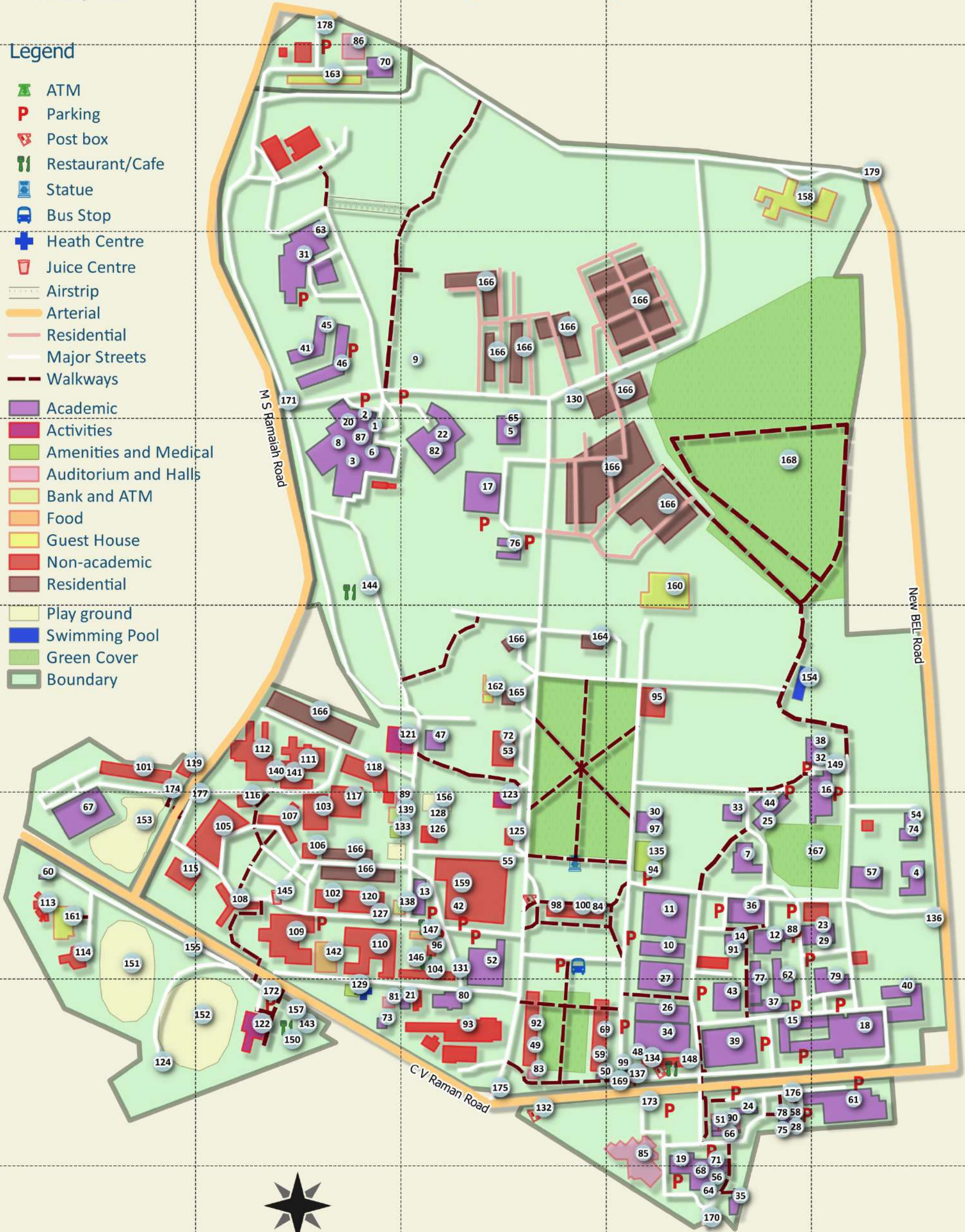
Time	Main Auditorium	Hall A	Hall B	Hall C
09:30-11:30	Parallel Session VII Biological Systems and Medicine Chair: Shinji Saito Keynote Talk: Anand Srivastava Invited Talk: Ramasubbu Sankararamakrishnan Invited Talk: Aditya Padhi Invited Talk: Prapasiri Pongprayoon Contributed Talk: Raj Kumar Sadhu Contributed Talk: Amar Krishna Gopinath	Parallel Session VII Computational Material Sciences Chair: Sai Gautam Gopalakrishnan Keynote Talk: Jayant K Singh Invited Talk: Sairam Mallajosyula Invited Talk: Krishan Kanhaiya Contributed Talk: Ravi C. Dutta Contributed Talk: Diksha Kadre Contributed Talk: Prashil Badwaik	Parallel Session VII ML/AI and Molecular Modeling Chair: Yun Hee Jang Keynote Talk: Sanjib Senapati Invited Talk: Saientan Bag Invited Talk: Tarak Patra Invited Talk: RS Swathi Contributed Talk: Maida Engels SE Contributed Talk: Arya Das	Parallel Session VII Materials and Biological Systems Chair: Supawadee Namuangruk Contributed Talk: Sayari Bhattacharya Contributed Talk: Rakesh K Vaiwala Contributed Talk: Pooja Sahu Contributed Talk: V N Ravi Kishore Vutukuri Contributed Talk: Pujarini Mahapatra Contributed Talk: Sayantan Maity
11:30-12:30	CONCLUSION SESSION – MAIN AUDITORIUM			
12:30-14:00	LUNCH/DEPARTURE			



Indian Institute of Science (IISc) Campus Map

Legend

- ATM
- Parking
- Post box
- Restaurant/Cafe
- Statue
- Bus Stop
- Heath Centre
- Juice Centre
- Airstrip
- Arterial
- Residential
- Major Streets
- Walkways
- Academic
- Activities
- Amenities and Medical
- Auditorium and Halls
- Bank and ATM
- Food
- Guest House
- Non-academic
- Residential
- Play ground
- Swimming Pool
- Green Cover
- Boundary



Map composed by Gubbi Labs | Map data: © Gubbi Labs and OpenStreetMap contributors

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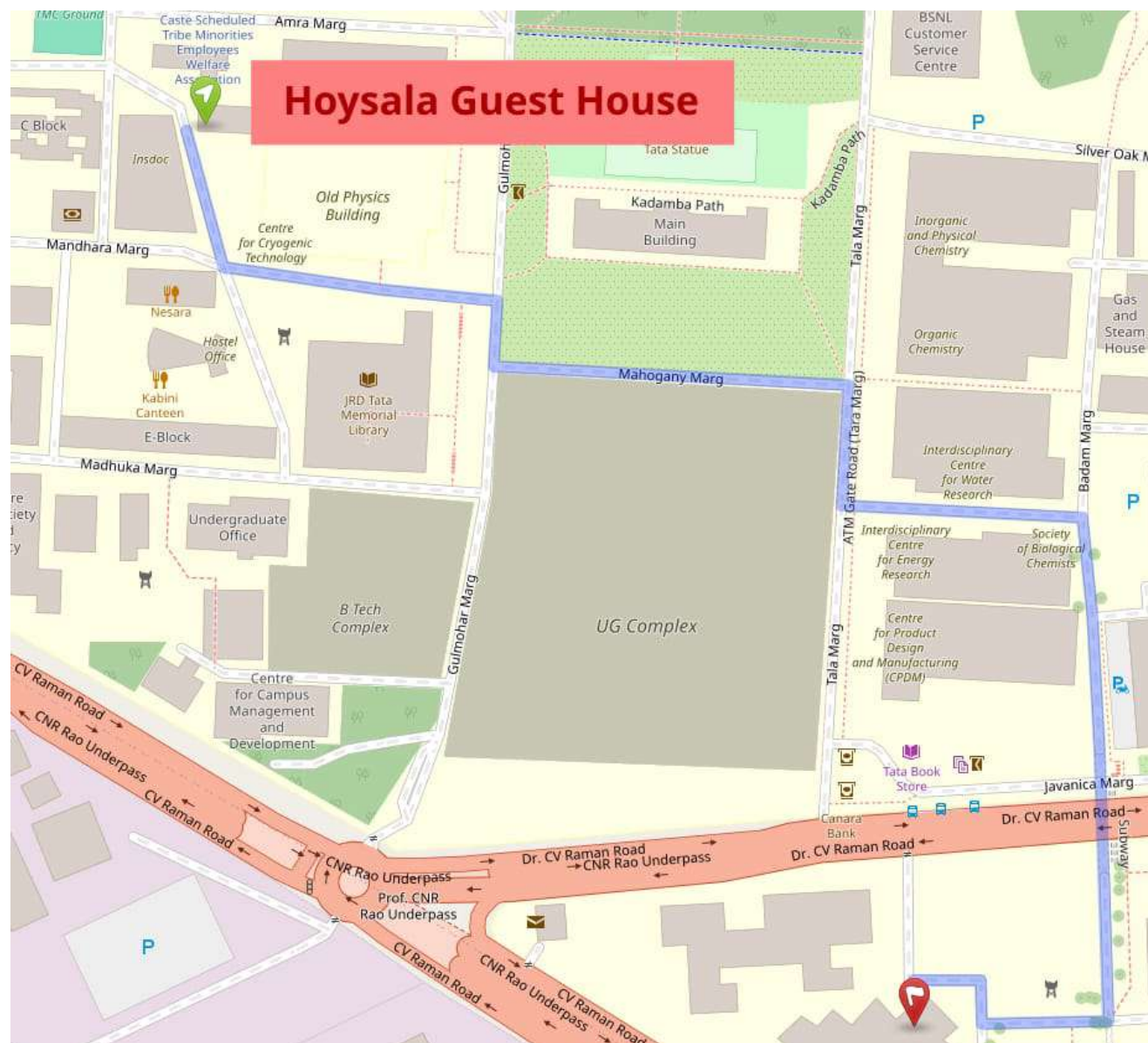
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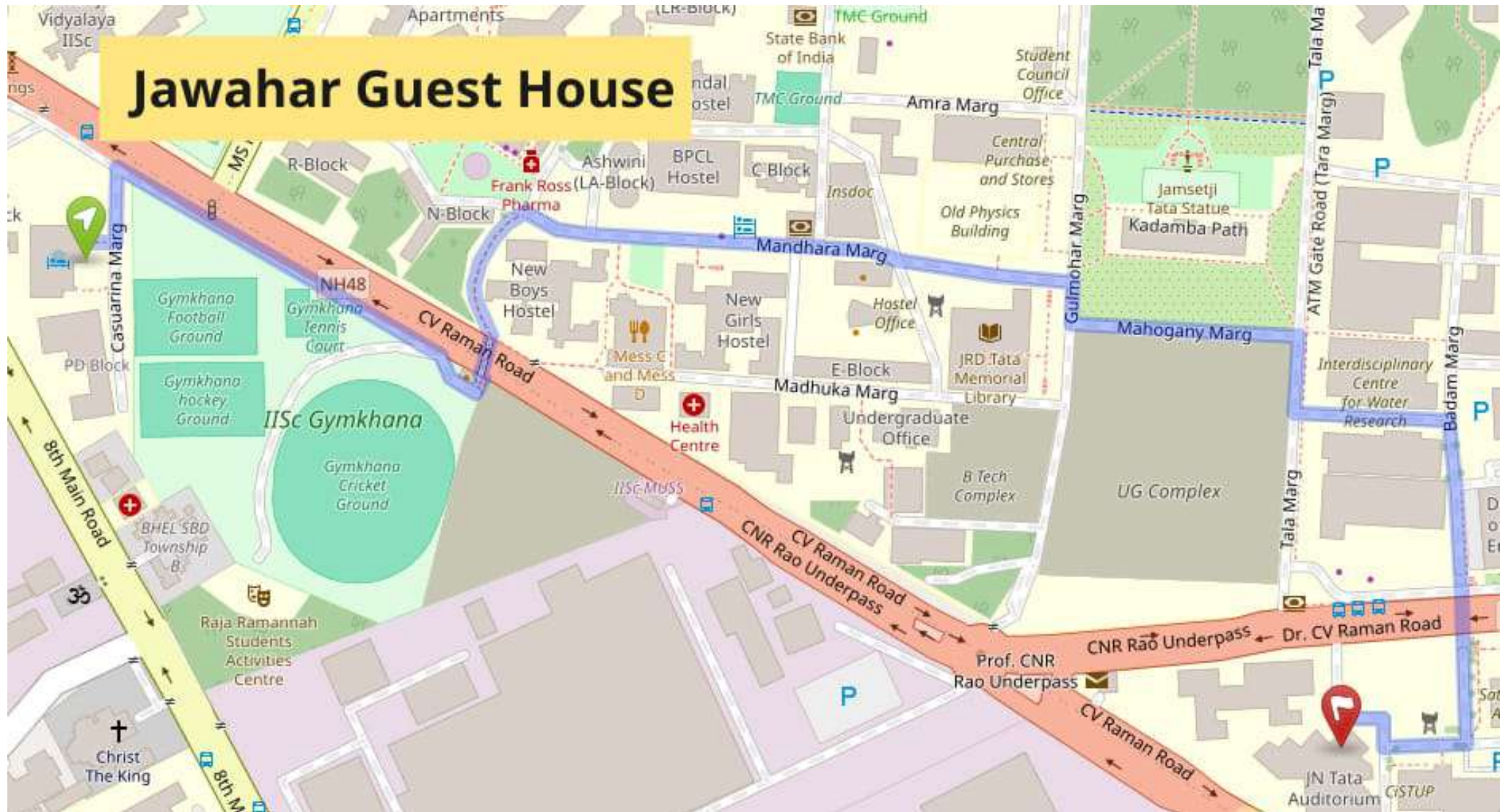
Directions from Hoysala Guest House to JN Tata Auditorium

Google Maps route map: https://www.google.com/maps/d/viewer?mid=1Pqyy0ENOPmadY_K6dX2X0TZqH2JHILE



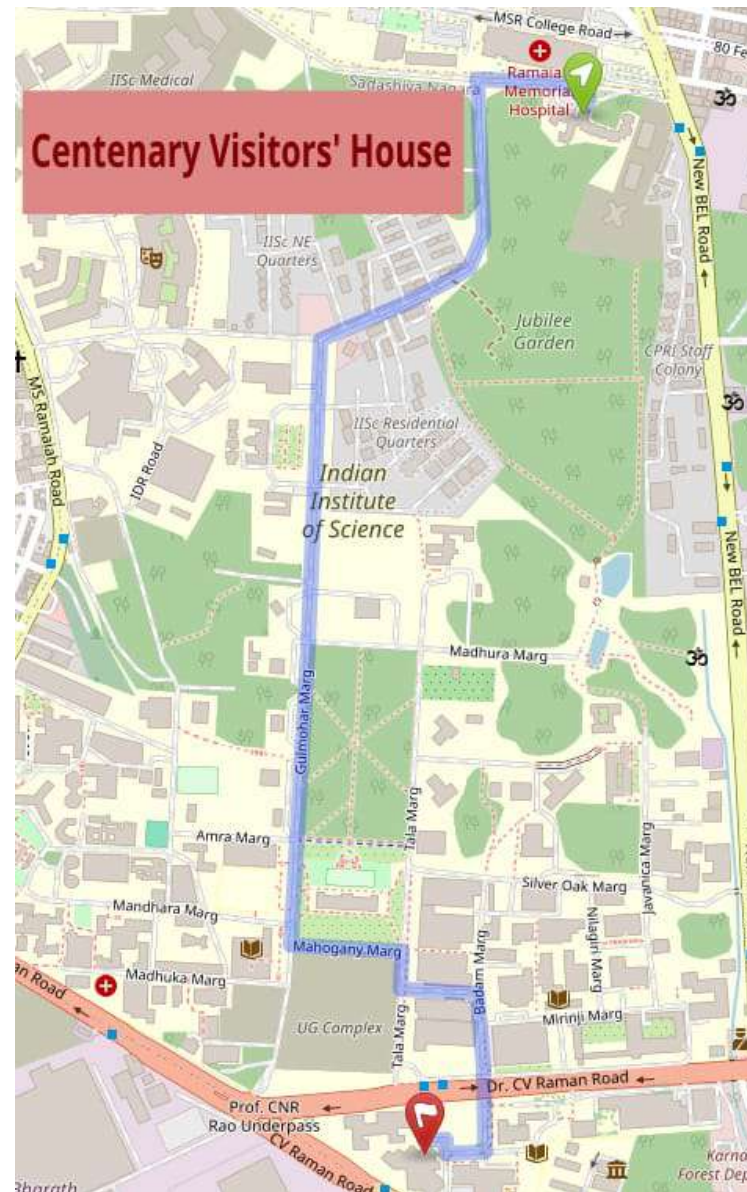
Directions from Jawahar Guest House to JN Tata Auditorium

Google Maps route map: https://www.google.com/maps/d/viewer?mid=1Pqyy0ENOPmadY_K6dX2X0TZqH2JHILE



Directions from Centenary Visitors' House to JN Tata Auditorium

Google Maps route map: https://www.google.com/maps/d/viewer?mid=1Pqyy0ENOPmadY_K6dX2X0TZqH2JHILE



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	Chaitanya Jitendra Shah	+91 8875050352	chaitanyasj@iisc.ac.in

Monte Carlo Simulations Probing Retention in Liquid and Supercritical Fluid Chromatography

J. Ilja Siepmann^{1,2}

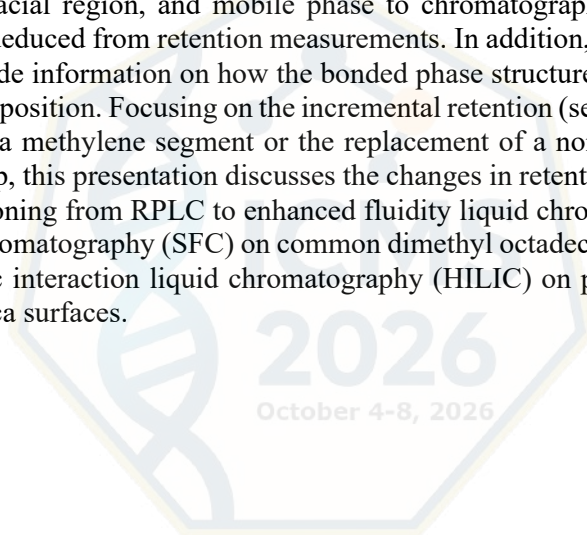
¹*Department of Chemistry and Chemical Theory Center, University of Minnesota - Twin Cities, Minneapolis, Minnesota 55455-0431, USA.*

²*Department of Chemical Engineering and Materials Science, University of Minnesota - Twin Cities, Minneapolis, Minnesota 55455-0132, USA.*

**Email: siepmann@umn.edu*

Abstract

Molecular simulations can reveal detailed mechanistic information on the contributions of bonded phase, interfacial region, and mobile phase to chromatographic retention that goes beyond what can be deduced from retention measurements. In addition, analyses of simulation trajectories can provide information on how the bonded phase structure respond to changes in the mobile phase composition. Focusing on the incremental retention (separation factor) arising from the addition of a methylene segment or the replacement of a non-polar hydrogen atom with a hydroxyl group, this presentation discusses the changes in retention and their molecular origins when transitioning from RPLC to enhanced fluidity liquid chromatography (EFLC) to supercritical fluid chromatography (SFC) on common dimethyl octadecylsilane (ODS) bonded phases to hydrophilic interaction liquid chromatography (HILIC) on polar bonded phases or chromatographic silica surfaces.



Integrative modeling approaches to characterize the dynamics of biomolecules

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Abstract

To fully understand biological functions, high-resolution biomolecular structures are required, which can be obtained through diverse experimental methods such as X-ray crystallography and, more recently, cryo-electron microscopy (cryo-EM) and computationally via AlphaFold3. While these techniques provide valuable structural insights, elucidating the dynamics of these biomolecules is also essential, given that some molecules display inherent structural flexibility through spontaneous large-domain motions. A thorough comprehension of such dynamics involves characterizing various conformational states at the atomic level. Raw experimental data from cryo-EM or high-speed atomic force microscopy (AFM) experiments consist of 2D images that represent specific views of a biomolecule, potentially capturing different conformational states, as each image may correspond to a distinct conformation. To bridge the gap between these 2D images and atomic models, simulation techniques can produce conformations in agreement with the observed data. We will introduce our efforts in developing these methods and discuss some of their applications.

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Domain organization in nanoscale phase-separated lipid vesicles

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Phase separation in multicomponent lipid membranes is generally understood in terms of line tension, which promotes domain coarsening and domain-induced budding in giant vesicles. Whether the same physical picture remains valid for nanoscale vesicles, however, is less clear because membrane curvature and elastic heterogeneity become increasingly important at small length scales. In this work, we use molecular dynamics simulations and continuum free-energy analysis to investigate domain organization in nanoscale phase-separated lipid vesicles. By resolving the coupling between vesicle morphology, domain localization, and membrane elastic properties, we identify a distinct energetic pathway that becomes accessible only at nanoscale dimensions. We find that demixing between liquid-ordered and liquid-disordered membrane regions is accompanied by solvent release and a morphological transition toward an oblate vesicle shape. In this geometry, the liquid-disordered domain preferentially occupies the equatorial rim, forming a band-like structure between liquid-ordered polar caps. Helfrich-based free-energy calculations show that this three-domain arrangement can be more stable than the conventional two-domain configuration below a characteristic vesicle size of approximately 50 nm. These results suggest that nanoscale membranes can access domain architectures that differ qualitatively from those observed in giant vesicles, owing to a shift in the balance between line tension and curvature elasticity. Our findings provide a physical framework for understanding lateral organization in small biological membranes, including exosome-sized vesicles.

How Do PAMs Talk to M4? Exploring Allosteric Communication Networks Through Molecular Dynamics Simulations

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Abstract

Positive allosteric modulators (PAMs) offer a promising approach for achieving selective modulation of muscarinic acetylcholine receptors by targeting sites distinct from the highly conserved orthosteric binding pocket. Despite considerable interest in M4-selective PAMs, the molecular basis by which these ligands influence receptor dynamics and long-range communication remains incompletely understood. In this study, molecular dynamics simulations were performed on membrane-embedded M4 muscarinic acetylcholine receptor systems bound to the orthosteric agonist iperoxo alone and in combination with the PAMs LY2033298 and VU0467154. Receptor structures obtained from experimentally determined complexes were prepared using established membrane simulation protocols and simulated in explicit POPC lipid bilayers. Structural and dynamical properties were characterized using trajectory-based analyses, including principal component analysis and Contact Map Analysis of Residue-Residue Associations (CAMERRA), to examine ligand-dependent changes in receptor motions and residue-residue communication patterns. By comparing orthosteric-only and PAM-bound systems, this work explores how allosteric ligand binding may influence communication pathways within the receptor and how structurally distinct PAMs may differentially affect the dynamic behavior of M4. This study illustrates how molecular dynamics simulations and contact network analysis can be used to investigate the dynamic basis of allosteric modulation and examine communication networks associated with allosteric receptor regulation.

Keywords: M4 muscarinic receptor; Positive allosteric modulators; Molecular dynamics simulations; Allosteric communication

ATP-Driven Asymmetric Gating and Lateral Cholesterol Entry in Human ABCA1: Insights from Multiscale Coarse-Grained Molecular Dynamics

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Abstract

ABCA1 is a critical ATP-binding cassette (ABC) transporter that mediates reverse cholesterol transport from peripheral macrophages to nascent high-density lipoprotein (HDL) particles, a process central to cardiovascular protection. Loss-of-function mutations in ABCA1 cause Tangier disease and familial hypoalphalipoproteinemia, yet the molecular mechanisms linking ATP binding to conformational rearrangements and lipid transport remain incompletely understood. Here, we present a comprehensive multiscale coarse-grained molecular dynamics study of full-length human ABCA1 in a physiologically relevant seven-component macrophage-like bilayer (POPC, POPE, POPI, POPS, POSM, LPC, and cholesterol), employing the Martini 2.2/ElNeDyn force field across ATP-unbound (5XJY) and ATP-bound (7TBW) states, accumulating 110 microseconds of aggregate simulation time.

ATP binding drives asymmetric closure of the nucleotide-binding domains (NBD distances: 21-23 Å in the unbound state versus 5-7 Å in the bound state), accompanied by a large-scale extracellular domain (ECD) rotation of approximately 28.8 degrees ($p = 0.005$) and stabilization of a cross-TMD salt bridge (Asp1645-Arg565) validated against published mutagenesis data. In the ATP-unbound state, we observe spontaneous intracavity cholesterol capture absent in all ATP-bound replicates, providing direct simulation evidence for a lateral entry mechanism gated by asymmetric TMD2 opening. Cholesterol flip-flop rates are significantly elevated in the unbound state (5.12×10^4 versus 3.79×10^4 events/sec, $p < 0.001$), consistent with an ATP-dependent lipid scrambling mechanism.

A constitutive phosphoinositide (POPI) annulus is identified that persists across both nucleotide states, suggesting a structural role in ABCA1 membrane organization independent of ATP status. Together, these findings provide a mechanistic framework for ATP-dependent lipid remodeling in ABCA1 and offer coarse-grained simulation insights into the conformational basis of cholesterol efflux and HDL biogenesis.^[1]

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pH-Dependent Free Energies and Molecular Mechanism of Insulin Fibrillation from Protonation Ensemble Statistics

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Abstract

Protonation equilibria play a central role in regulating protein aggregation, yet connecting protonation-state fluctuations to pH-dependent free energies and molecular mechanisms remains a major challenge in computational biophysics. Here, we present a unified framework that links protonation ensembles, thermodynamic stability, and atomic mechanisms using constant-pH molecular dynamics (CpHMD).

First, we introduce PRIME (Protonation-state Reweighting in Multi-pH Ensembles), a statistically optimal estimator that extracts pH-dependent free energies directly from CpHMD simulations. By utilizing the full protonation-state distributions across multiple pH conditions, PRIME eliminates discretization errors associated with conventional thermodynamic integration and utilizes the entire sampled protonation distribution rather than just its first moment.

Using this framework, we investigate the pH-dependent fibrillation of human insulin. Within the semi-grand canonical ensemble of protons, we establish a direct relationship between protonation statistics and pH-dependent free-energy differences between native and fibrillar states. Application to insulin assemblies reveals a non-monotonic free-energy landscape with a stability crossover near pH 5.5, consistent with experimental observations that fibrillation is favored under acid and weakly acidic conditions. Larger fibrillar assemblies exhibit increasingly favorable free energies, indicating protonation-mediated stabilization strengthens with self-association.

To uncover the molecular origin of this behavior, we characterized protonation equilibria from native insulin to extended fibrils. Whereas native and fibrillar folded monomers exhibit largely independent titration behavior, self-association induces strong electrostatic coupling between neighboring glutamate residues aligned along the fibril axis. These interactions generate cooperative, multistep protonation equilibria, spatially correlated charge distributions, and collective electrostatic frustration that cannot be explained by solvent accessibility alone. The resulting charge redistribution stabilizes fibrillar assemblies at low pH while progressively weakening inter-monomer cohesion upon deprotonation.

Together, these results establish a direct connection between protonation-state statistics, pH-dependent free energies, and atomistic mechanisms. More broadly, they provide a foundation for studying pH-dependent biomolecular equilibria, where self-association represents only one case within a wider class of protonation-coupled processes.

Miniature work-to-work converter engine powered by motor protein

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Abstract

Designing a miniature microscale engine that can override the role of thermal fluctuations has remained elusive and is an important open challenge. Here, we provide the design and theoretical framework for a unique information-based engine—a work-to-work converter—comprising a submicron-sized bead and motor protein-microtubule (MT) complex in an optical trap setup. We demonstrate how, by implementing a simple motor-protein state-dependent feedback protocol of the optical trap stiffness, this engine is able to harness and convert the movement of a motor protein into work output. Unlike other conventional microengines, the fidelity and performance of this engine are determined by the stochasticity of motor (un)binding characteristics. We obtain an analytical form of the work distribution function, average work output, and average power output, providing quantitative predictions for engine performance which are validated by stochastic simulations. Remarkably, the average work output per cycle is at least an order of magnitude higher than the thermal fluctuations and supersedes the performance of other microscale engines realized so far.^[1]

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How Do Additives Promote Gas Hydrate Nucleation? Mechanistic Insights from Molecular Simulations and Nucleation Theory

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Abstract

Gas hydrate nucleation is a complex self-assembly process involving the cooperative organization of water and guest molecules into an ordered crystalline structure. Recent advances in molecular simulations and nucleation theory have significantly improved our understanding of hydrate nucleation, revealing the molecular structures, intermediate states, and kinetic pathways involved in nucleus formation. An intriguing question arises when chemical additives are introduced. Intuitively, an additional molecular species could disrupt molecular ordering, alter local structure, or hinder the propagation of the hydrate growth front. Yet many additives are observed to accelerate hydrate formation. Understanding how additives promote nucleation despite these apparent challenges remains a fundamental question in hydrate science.

In this lecture, we present a mechanistic framework^[1-3] that combines molecular dynamics simulations, mean first-passage time (MFPT) analysis, and the Becker–Döring kinetic model to quantify additive effects on gas hydrate nucleation. Within this framework, nucleation kinetics can be decomposed into three key contributions: the thermodynamic driving force, the hydrate–liquid interfacial free energy, and the molecular attachment kinetics governing cluster growth.

Using CO₂ hydrate nucleation as a model system, we investigate the effects of various additives, including urea, cysteine, and methionine. Our results show that enhanced nucleation rates can arise from distinct molecular mechanisms. While some additives primarily increase the thermodynamic driving force, others reduce the interfacial free-energy barrier or accelerate molecular attachment to growing hydrate clusters. These findings demonstrate that additives do not promote hydrate nucleation through a universal mechanism; rather, their effectiveness depends on how they modify the thermodynamic and kinetic processes underlying nucleation. The insights gained from this work provide a foundation for the rational design of next-generation hydrate promoters.

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Exploring the Ion Conduction Mechanism of Glass Solid-State Electrolytes

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Abstract

Inorganic glass solid-state electrolytes (IGSSEs) have emerged as promising materials for next-generation all-solid-state lithium batteries because of their remarkable room-temperature ionic conductivity. However, the microscopic mechanism behind such superionic transport remains unclear. A long-standing debate centers on the “paddlewheel effect,” which proposes that lithium ion diffusion is assisted by the rotational motion of surrounding polyanions, though evidence for this mechanism has been inconclusive. In this talk, I will present a systematic computational framework combining large-scale machine learning molecular dynamics (MLMD) simulations with hop function analysis to investigate ion conduction in IGSSEs. A machine learning interatomic potential was developed for model systems of $\text{Li}_x\text{AlCl}_{3+x}$ ($x = 0.25\text{--}3$), accurately reproducing the experimentally observed non-monotonic composition dependence of lithium-ion conductivity, with a maximum at $x = 1$. Detailed analysis reveals that lithium transport occurs mainly through cascading hopping events rather than paddlewheel-like motions. We extend this approach to different types of IGSSEs including Li_3PS_4 and NaTaOCl_4 . This work provides mechanistic insight into ion transport in inorganic glass electrolytes and demonstrates how machine learning-driven molecular simulations can uncover complex diffusion behaviours in disordered materials.

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First-Principles Insights into Stable and Sustainable Perovskites for Energy and Optoelectronic Applications

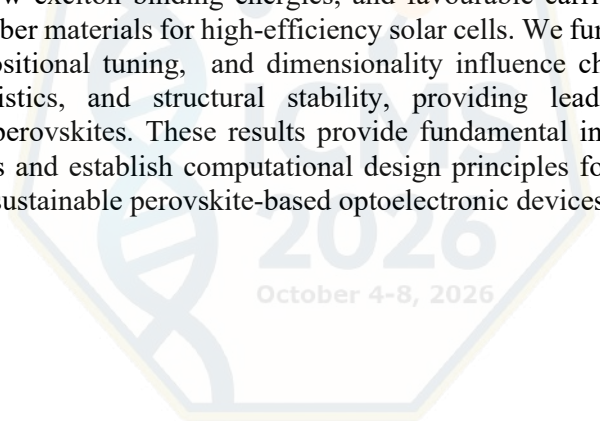
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Abstract

Perovskite materials have emerged as a versatile class of semiconductors for next-generation optoelectronic and energy-conversion technologies owing to their exceptional optical absorption, tunable electronic properties, and defect tolerance. In this talk, I will present our recent first-principles investigations aimed at designing environmentally benign and chemically stable perovskite systems for photovoltaic applications. Using density functional theory combined with many-body perturbation approaches (GW) and the Bethe-Salpeter equation, we explore the structural, electronic, optical, excitonic, and transport properties of a variety of all-inorganic perovskites. Our studies reveal that several chalcogenide based perovskites exhibit direct band gaps spanning the visible and near-infrared regions, strong optical absorption, low exciton binding energies, and favourable carrier mobilities, making them promising absorber materials for high-efficiency solar cells. We further demonstrate how structural and compositional tuning, and dimensionality influence charge transport, light-harvesting characteristics, and structural stability, providing lead-free alternatives to conventional halide perovskites. These results provide fundamental insights into structure–property relationships and establish computational design principles for the development of efficient, stable, and sustainable perovskite-based optoelectronic devices.



Functionalization of Nanomaterials for Hydrogen Storage Applications: A Multiscale Simulation Study

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Abstract

Hydrogen fuel offers a sustainable energy option; it has a high energy density—about three times that of fossil fuels.^{1,2,3} In our work, we investigated the chemical functionalization of boron nitride nanotubes (BNNTs) and transition metal doping of phosphorene nanosheets (PNS), to enhance their adsorption properties, with a particular focus on hydrogen storage applications. In this study, a multiscale simulation study combining density functional theory (DFT), ab initio molecular dynamics (AIMD), and grand canonical Monte Carlo (GCMC) is presented. Pristine BNNTs were functionalized with amine, amide, imine, and carboxylic groups. The electronic properties, charge density difference, and electron localization function of the functionalized BNNTs were studied. AIMD was used to determine the thermal stability of functionalized BNNT and the desorption temperatures, while GCMC was used to study the pressure-temperature effects on adsorption and adsorption isotherms. The amine-BNNT had the highest capacity of 5.6 wt% and volumetric capacity of 23.86 g/L at 250 K and 100 bar. The transition-metal doped phosphorene sheets (TM-PNS), improved the surface chemistry and electronic structure for Kubas-type adsorption. Adsorption energies were obtained using DFT, and charge density differences, vibrational properties, and d-band theory were used to analyze H₂ adsorption on the functionalized systems and understand the adsorption mechanisms at the atomic scale. Our results showed that functionalization significantly improved the interaction between hydrogen molecules and the host materials (BNNT and PNS), primarily through induced dipole interactions and charge redistribution. The TM-PNS binds H₂ through Kubas-type interaction with an average binding energy of 17.45 kJ/mol and 10.92 wt%, the strong hybridization, and de-localized states of TM-PNS improved electron mobility. Phonon spectra and vibrational analyses were used to confirm the dynamical stability and mechanical properties of the modified structures.¹ These studies provided fundamental insights into the role of surface functionalization in modifying the physicochemical properties of low-dimensional nanomaterials and offer a viable pathway for designing next-generation materials.

Keywords: BNNT, PNS, doping, H₂ adsorption, density functional theory, AIMD, GCMC

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Above the Core: Unraveling Top-Sitting Interactions of Heavy Metals with Porphyrins: DFT Study

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Abstract

Porphyrins are attractive molecular platforms for sensing applications due to their exceptional chemical stability, redox activity, and tunable electronic properties.^{1,2} Inspired by our previous investigations of transition metal interactions with *N*-confused tetraphenylporphyrin (NCTPP)³, we extended this study to explore its potential for toxic heavy-metal sensing. In the present work, density functional theory (DFT) calculations were employed to investigate the interactions of NCTPP and its metal complexes (M–NCTPP) with environmentally hazardous heavy metal ions, including Hg²⁺, Pb²⁺, and Cd²⁺. Geometry optimization and electronic structure analyses reveal a preferred atop-sitting coordination mode, highlighting the role of non-planar metal macrocycle interactions in stabilizing the complexes. Binding energetics, structural parameters, and simulated spectroscopic properties indicate strong metal-ion affinity and high thermal stability. The intrinsic water insolubility and structural rigidity of NCTPP-based systems further enhance their suitability for operation in organic media. These findings provide molecular-level insights into the sensing mechanism of NCTPP derivatives and demonstrate their potential as robust, cost-effective platforms for selective heavy-metal detection, ion-selective membranes, and related environmental monitoring applications.

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Insights into the Mechanism of NaCl Nucleation from Aqueous Solutions: *The Interplay between Aggregation, Crystallisation, and Dehydration*

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Abstract

Crystallisation is a widely used unit operation in chemical industries, especially in the production of fertilizers, food additives, and medicines. The first step in the crystallisation process is crystal nucleation. It has been established that this step controls the quality of the product as well as plays a crucial role in determining the dominant polymorph in the final product. Thus, understanding crystal nucleation is of utmost importance to obtain greater control over the product quality. However, observing nucleation events in experiments is extremely difficult as the time and length scales at which nucleation occurs are not experimentally accessible. Molecular simulations, on the other hand, are free of such spatio-temporal constraints and provide a potent alternative to investigate the nucleation mechanism at the molecular level.

In spite of such a significant advantage, simulating crystal nucleation from a solution is highly non-trivial. The slow diffusion of solute molecules to reach the crystal-solution interface makes the nucleation process exceedingly slow and hence challenging to investigate in an MD simulation. Another technical challenge is to maintain the supersaturation during crystal growth. To overcome these challenges, the Molecular Theory of Nucleation from dilute phases¹ was developed in our group. Apart from bypassing the aforementioned challenges, the Molecular Theory also enables the modelling of non-classical nucleation mechanisms by including crystallinity, i.e., the crystalline portion inside a nucleus, as a collective variable along with the nucleus size. In this work, we borrow the elements of the Molecular Theory to systematically investigate the crystal nucleation of NaCl from an aqueous solution. In our simulations, we find that the degree of hydration of a nucleus is a slow degree of freedom that affects the ion arrangement in a nucleus and, hence, the crystallinity, necessitating its inclusion as an independent collective variable to characterise a nucleus. Incorporating solvation as a third degree of freedom reveals a rich three-dimensional free energy landscape in which crystallinity emerges only beyond a threshold nucleus size. The free energy landscapes disclose a continuous transition in nucleation mechanism from 1-step to 2-step as the supersaturation increases toward the spinodal. The estimates of critical nucleus size determined through committor analysis are substantially smaller than the estimates from prior forward-flux sampling simulations². This discrepancy is attributed to the presence of water molecules in the nuclei formed during the unbiased simulations, making the nucleus unstable and pushing the critical nucleus estimates to higher values. Our simulations establish that the reaction coordinate for NaCl crystal nucleation from solutions is at least three-dimensional, with broad implications for computational studies of crystallisation kinetics of solutes from their solutions.

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Decoding Chemical-Scale Mechanical Heterogeneity in Proteins and Nucleic Acids with Physics-Based Machine Learning

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Abstract

In understanding the chemical origin of biomolecular functionality, going beyond a purely structural perspective has become essential given the availability of AI tools. A key question is how do specific functional properties arrive from the sequence composition and molecular details. In this talk, our development of structure-mechanics statistical learning (SMSL) framework that integrates all-atom molecular dynamics simulations, machine learning, and graph theory is discussed. Even under similar biomolecular structures, diverse mechanical properties can emerge at the chemical scale. Findings enabled by this approach include the mechanical relay system in protein allostery, functional conformational changes, mechanical codes in transcription regulatory DNA sequences, mechanical reorganization in G-quadruplexes upon inhibitor binding, and protein-drug interactions involving an intrinsically disordered region.^[1-9] Implications for drug development targeting physiologically important biomolecules are addressed in terms of the SMSL framework.

October 4-8, 2026

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Understanding of humidity-induced phase transition in CALF-20 from machine learning potential

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Abstract

Calgary Framework-20 (CALF-20) is an attractive metal organic framework that has a high selectivity toward adsorbing CO₂ even under humid conditions. However, a phase transition from open to closed pore was experimentally confirmed with the rise of humidity, which eventually blocks CO₂ penetration. Although this is a very interesting phenomenon, the molecular-level understanding of how H₂O induces the phase transition is still a mystery. To account for the competitive interaction between CALF-20 and H₂O as well as water clustering, we developed a machine learning potential (MLP) that achieves density functional theory accuracy while maintaining high scalability. To understand the driving force for phase transition, we extracted the key water configurations that stabilize the closed pore phase using MLP-based molecular dynamics simulations. Moreover, metadynamics sampling was used to clarify the critical H₂O binding geometries near the Zn metal center for CALF-20 at 298 K. These configurations exhibit long lifetimes in the closed pore phase and are critical for stabilizing this phase, which is in agreement with the previously reported X-ray diffraction experimental studies.^[1]

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Phonons, Paddles, and Percolation Pathways: Mapping Cation Transport via Machine Learning

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Abstract

Optimizing solid-state electrolytes requires a comprehensive atomistic understanding of how the surrounding lattice matrix couples with mobile ions to break traditional diffusion trade-offs. While *ab initio* molecular dynamics yields accurate mechanistic snapshots, its strict spatiotemporal limits often obscure the long-range, correlated lattice dynamics and low-frequency fluctuations that dictate macroscopic transport. In this talk, we show how Machine Learned Interatomic Potentials (MLIPs) circumvent these limitations, unlocking quantum-accurate, nanosecond-scale simulations across both crystalline and amorphous chemically complex systems. Using MLIPs, we probe multiscale diffusion pathways across four distinct structural paradigms: antiperovskite crystals, thiophosphates, amorphous oxynitrides, and metal-organic framework glasses. We systematically disentangle how local framework flexibility modulates free-energy activation barriers to accelerate ion migration. Specifically, we examine the highly correlated, phonon-assisted lithium-ion hopping in thiophosphates, where specific lattice vibrational modes act as transient structural gates. We contrast this with the rotational, polyanionic "paddle-wheel" effect in antiperovskites, and further extend these transport principles to glassy media to reveal how topological disorder modifies percolation pathways. Ultimately, our findings highlight MLIPs as a powerful toolkit for mapping the delicate interplay between lattice dynamics and structural frustration, establishing universal design rules for next-generation solid-state energy storage materials.

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AI-augmented MD for protein native conformational ensemble modeling

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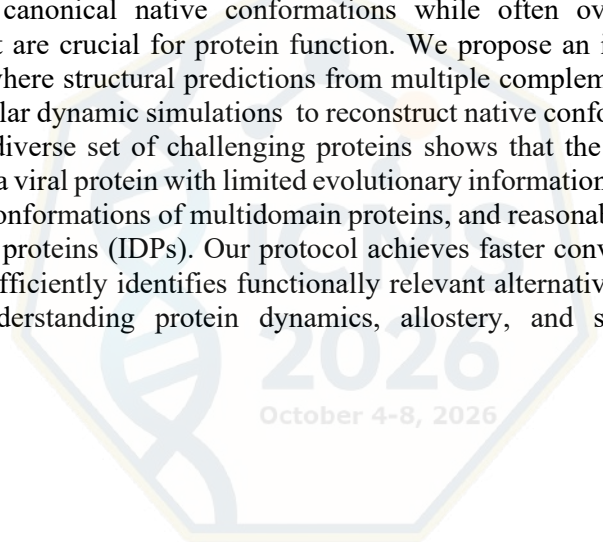
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Abstract

Recent advances in artificial intelligence (AI) have revolutionized protein structure prediction with deep learning models achieving unprecedented accuracy and speed. However, no single AI framework consistently performs optimally across all protein targets and current methods excel in predicting canonical native conformations while often overlooking alternative metastable states that are crucial for protein function. We propose an integrated hybrid AI–physics framework where structural predictions from multiple complementary AI models are augmented in molecular dynamic simulations to reconstruct native conformational ensembles. Validation across a diverse set of challenging proteins shows that the protocol can recover correct native fold of a viral protein with limited evolutionary information, identify functionally relevant alternative conformations of multidomain proteins, and reasonably model challenging intrinsically disorder proteins (IDPs). Our protocol achieves faster convergence compared to traditional MD and efficiently identifies functionally relevant alternative conformations with implications for understanding protein dynamics, allostery, and structure-guided drug discovery.



MembraneFinder: A Simulation-Trained Framework for Membrane Detection and Analysis in Cryo-EM images

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Abstract

Automated and accurate lipid membrane detection in cryo-electron microscopy (cryo-EM) images is essential for the detailed structural characterization of both biological and model membranes. Existing deep-learning tools often fail across variable imaging conditions and require tedious parameter tuning, model retraining, and manual annotation. To address these limitations, we present MembraneFinder, a comprehensive framework for lipid membrane detection trained exclusively on physics-informed synthetic data. The complete framework is split across three integrated pipelines. First, the synthetic data generator utilizes molecular dynamics simulations to produce large-scale batches of synthetic cryo-EM images. The synthetic datasets span variable imaging conditions, noise distributions, vesicle sizes, and morphologies. They also include multi-lamellar vesicles with realistic spacing and angular deformations in the overall shape of the membrane. Crucially, the pipeline automatically generates precise ground-truth masks for these simulated structures, completely eliminating the need for manual annotation. Second, the model training and inference pipeline utilizes these image-mask pairs to train a neural network based U-Net architecture for binary membrane segmentation. When validated against public EMPIAR repositories and diverse in-house samples, the model achieves high detection rates outperforming commonly used software packages developed for general analysis of cryo-EM images. Finally, the analysis pipeline extracts quantitative structural insights from the segmented outputs, allowing us to measure not only readily visible features like membrane shape and curvature but also local bilayer properties like thickness which can vary spatially as a result of interactions with proteins and other particles of interest.

Electric Double Layers as Active Interfacial Phases Governing Electron Transfer

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Abstract

Electric double layers (EDLs) govern charge storage, interfacial electric fields, and electrochemical reactivity, yet their collective molecular response to electrode charging remains poorly understood under realistic aqueous conditions. In this talk, I will present a theoretical framework that reinterprets the EDL as a system exhibiting interfacial phase transitions, where collective water reorganization and ion condensation give rise to characteristic capacitance anomalies and emergent electrochemical behavior.

Building on this perspective, I will discuss how cation-dependent EDL structures fundamentally regulate interfacial electron transfer (ET) pathways, including cation-coupled electron transfer and homogeneous cocatalytic effects of alkali metal cations. To quantitatively investigate these dynamics, we developed a semiclassical multistate quantum dynamics method based on thermalized Gaussian wavepackets, enabling real-time simulations of finite-temperature electron transfer with explicit decoherence and bath effects.

Together, these results establish a unified molecular framework connecting interfacial thermodynamics, interfacial ionic structures, and electron transfer dynamics, capturing both collective EDL structure and electrochemical reactivity at an atomistic level.

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Understanding Rock-Crude Oil Interactions for Enhanced Oil Recovery Using Molecular Simulations

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Abstract

The efficiency of enhanced oil recovery (EOR) is strongly influenced by the molecular-level interactions between crude oil components and reservoir rock surfaces. The deposition of heavy fractions such as asphaltenes leads to wettability alteration, pore blockage, and reduced oil mobility, posing significant technical and economic challenges. In our work,^[1-6] molecular dynamics simulations are employed to systematically investigate the structural and energetic behavior of crude oil components—including saturates, aromatics, heavy oil, and model asphaltenes—on representative mineral surfaces such as calcite, silica, and mica.

Potential of mean force calculations (PMF) reveal that asphaltenes exhibit significantly stronger adsorption than saturates, primarily due to heteroatom-mediated interactions. Polar functional groups (oxygen- and nitrogen-containing) enhance adsorption via electrostatic and hydrogen-bonding interactions, whereas sulfur-containing species show weaker affinity. The nature of the mineral surface plays a critical role: calcite exhibits the highest adhesion, followed by mica and silica. Dispersion interactions dominate in calcite and silica systems, while both electrostatic and dispersion contributions are significant in mica systems.

Interfacial structuring reveals the formation of a dense adsorbed layer near the surface, with preferential adsorption of aromatic components on calcite and mica, and aliphatic components on silica. Molecular orientation is governed by the interplay between aromatic core interactions and steric effects of aliphatic chains. Additionally, competition between solvent and asphaltenes, along with hydrogen bonding and configurational energy, dictates adsorption selectivity and desorption barriers.

These insights provide a mechanistic framework for designing targeted solvents and additives to improve oil displacement and enhance EOR efficiency.

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Density functional theory-based investigation of adsorption, permeation and desorption of hydrogen isotopes in Fe-Cr alloy of varied compositions

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Abstract

A fundamental understanding of hydrogen behavior in Fe–Cr alloys is critical for mitigating hydrogen-related challenges in fusion and fission reactor environments¹⁻³. Extensive calculations are performed using plane-wave density functional theory to investigate the interaction and dynamics of hydrogen isotopes in model bcc Fe–Cr system. The hydrogen dissociative adsorption on Fe–Cr surfaces is found to be exothermic, whereas absorption into bulk sites is shown to be endothermic. The findings reveal that the tetrahedral-site absorption energies for hydrogen become increasingly endothermic with rising Cr concentration. NEB calculations show that the predicted diffusion barriers of hydrogen isotopes increase with Cr content and thus reduced the permeation. The computed diffusion, permeation, and solubility trends agree with the experimental results. The analysis of hydrogen isotopes highlights the role of zero-point energy in governing the desorption kinetics of hydrogen.

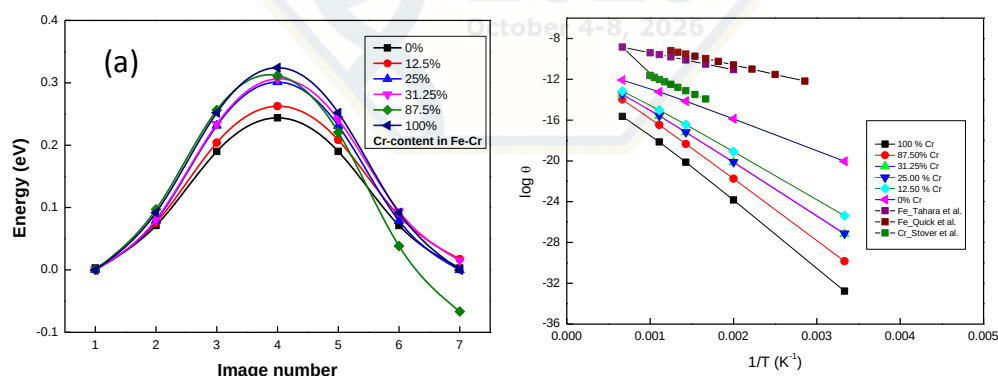


Figure:(a) Energy profile for H diffusion from T-T site with variation in the Cr concentration (b) Plot of calculated permeability coefficients (θ , $\text{mol.m}^{-1}.\text{s}^{-1}.\text{Pa}^{-0.5}$) of H at different temperatures with variation in the Cr content in Fe-Cr system.

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Electric Double Layer Structure in Concentrated Aqueous Solution

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Abstract

Toward tailored electrocatalysis, significant attention has been directed to the electrode-electrolyte interface. The electric double layer provides a crucial microenvironment for electrochemical reactions. However, its atomic-scale structure remains unresolved, particularly for non-dilute electrolyte concentrations relevant to practical systems. A notable example is the camel-to-bell shape transition in the capacitance curve, where two peaks merge as the concentration increases, which is still poorly understood at the molecular level. Herein, using mean-field quantum mechanics/molecular mechanics simulations under well-controlled bulk electrolyte concentrations, we elucidate the electric double layer structures and their phase transitions, which give rise to capacitance peaks.^[1] The predicted transition potentials match the experimental peak positions. We observe collective water reorientation in the cathodic region and anion surface condensation in the anodic region, which are also validated by in situ spectroscopy. Finally, we construct an electric double layer structural phase diagram to provide detailed insight into the electric double layer microenvironment. This work presents a valuable framework for the design of improved interfaces.

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Understanding Catalytic Applications and the Stability of Single-Atom Catalysts

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Abstract

Designing cost-effective and efficient electrocatalysts for water splitting and carbon dioxide reduction is key to reducing our dependence on fossil fuels and developing sustainable energy conversion technologies.^[1] Recent progress in computational multiscale modeling of solvent and electrolyte environments has created unprecedented opportunities to study the activity, selectivity, and stability of catalytic materials within a first-principles framework.^[2] In this presentation, I will discuss the applications of multiscale theoretical approaches developed to understand the underlying chemistry governing the efficiency of single-atom catalysts for sustainable energy applications.^[3-5] Particular attention will be paid to the computational methods that incorporate the effects of electrode potential, pH, solvent, and electrolyte to accurately represent the electrocatalytic reaction mechanisms. Selected applications of these methods to the screening and design of electrocatalysts for water splitting, CO₂, and O₂ reduction reactions will be presented. The developed computational framework has enabled the identification of promising catalytic materials with low thermodynamic overpotentials.^[6-7] The favorable reaction kinetics are fed into microkinetic models to understand the turnover frequencies and enhanced electrochemical stability. These studies not only provide the mechanistic details of catalytic activity but also establish predictive design principles for rational discovery of new electrocatalysts for sustainable energy applications.

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Water-Mediated Stabilization of Oxyl Radicals as Driving Force for the Oxygen Evolution Reaction

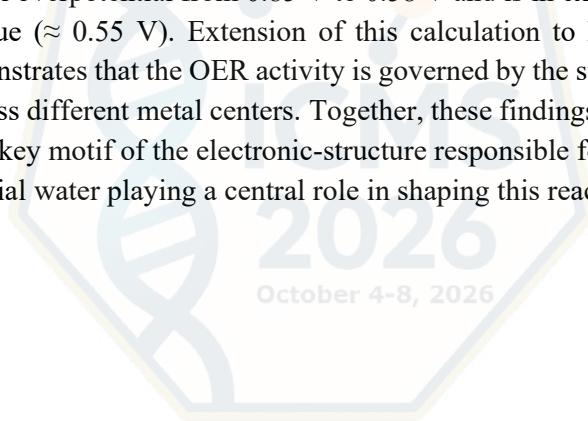
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Understanding the influence of interfacial water on the energetics of the oxygen evolution reaction (OER) remains a central challenge in oxide electrocatalysis. Here, using Mn_3O_4 as a model system, we show that the explicit inclusion of interfacial water fundamentally alters both the reaction pathway and electronic structure of key oxygen intermediates. First-principles calculations incorporating explicit networks of water molecules revealed that the interfacial water layer enhances the metal–oxyl character by selectively weakening the axial metal–oxygen (M–O) bond while suppressing over-oxidation of the metal center. This water-induced electronic reorganization lowers the O–O coupling barrier from 2.08 eV to 1.81 eV. This reduces the theoretical overpotential from 0.85 V to 0.58 V and is in excellent agreement with the experimental value (≈ 0.55 V). Extension of this calculation to heteroatom-substituted systems further demonstrates that the OER activity is governed by the strength of the axial M–O σ interaction across different metal centers. Together, these findings pinpoint the axial M–O σ interaction as a key motif of the electronic-structure responsible for controlling the OER activity, with interfacial water playing a central role in shaping this reactivity.



Nonlinear Vibrational Spectroscopy of Aqueous Surfaces and Interfaces from a Combination of Computational Approaches

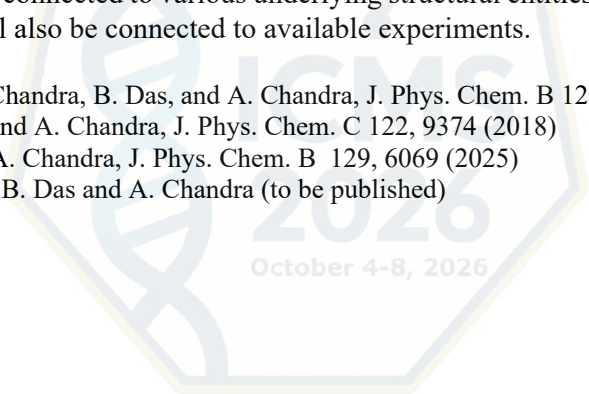
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The structure and dynamics of surfaces and interfaces can be obtained through second and fourth order techniques such as one-dimensional vibrational sum frequency generation (1D-VSFG) and the corresponding two-dimensional (2D-VSFG) spectroscopic techniques, respectively. We will present computational studies of these higher order vibrational spectroscopy using a combination of methods such as molecular dynamics simulations, quantum calculations, and machine learning methods. Specifically, we will present calculations of 1D-VSFG and 2D-VSFG spectra for a variety of aqueous surfaces and interfaces.^[1-4] The spectral results will be connected to various underlying structural entities and dynamical modes of the systems and will also be connected to available experiments.

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MHAT Reactivity in Engineered Metalloenzymes

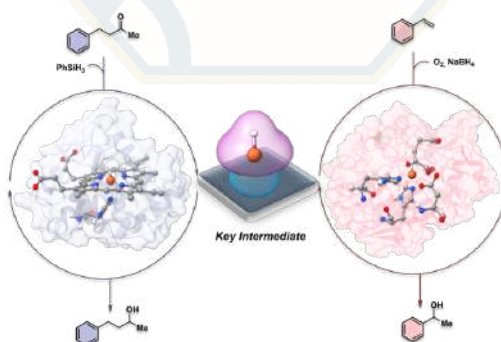
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Abstract

Metal–hydride (M–H) intermediates play pivotal roles in a wide range of catalytic transformations. While natural enzymes rarely exploit M–H reactivity, recent advances in protein engineering have demonstrated that repurposed scaffolds can access entirely novel catalytic regimes. Ward recently repurposed myoglobin into a catalyst capable of performing metal–hydrogen atom transfer (MHAT) based chemistry capable of carrying out a ketone reduction.^[1a] Chen reported another repurposed non-heme-based oxygenase undergoing Mukaiyama hydration of styrene derivatives.^[1b] However, despite the importance of M–H intermediates, the molecular determinants governing their formation and reactivity within biological scaffolds remain poorly understood. In this regard, we have performed multiscale computational investigations of Fe–H intermediates, providing a comprehensive molecular framework for understanding the generation and reactivity of Fe–H intermediates in engineered proteins and elucidating how electrostatic environments and ligand coordination modulate the balance between MHAT and hydride-transfer pathways. Our work integrates a rigorous computational strategy that combines extensive molecular dynamics (MD) simulations of various intermediates with quantum mechanics/molecular mechanics (QM/MM) calculations to capture key electronic and structural features. In the talk, I will explain our recent efforts in understanding the reactions shown in the Scheme below.^[2]



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Network Principles of Excitation Energy Transfer in Photosynthetic Supercomplexes

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Abstract

Photosynthetic supercomplexes achieve near-unity quantum efficiency despite their structural complexity, energetic disorder, and competing relaxation pathways. Understanding how efficient excitation energy transfer (EET) emerges from these large molecular assemblies remains a major challenge for molecular simulation. In this work, we develop structure-based excitonic models for the Photosystem II (PSII) and Photosystem I–LHCI (PSI–LHCI) supercomplexes by combining effective Hamiltonians with multiscale open quantum dynamics. To extract the essential transport mechanisms from these high-dimensional systems, we introduce network-theoretical approaches that map EET dynamics onto coarse-grained kinetic networks and statistically characterize their structural organization under energetic disorder. Our simulations reveal that efficient light harvesting is governed by hierarchical network architectures, where rapid local equilibration is coupled to robust long-range transport through a small number of persistent pathways. For PSII, the network analysis further uncovers a pseudo-one-dimensional transport topology and an optimized free-energy landscape that together alleviate unfavorable entropic effects while maintaining the energetic requirements for photochemistry. For PSI–LHCI, statistical analysis demonstrates that redundant and disorder-resistant transport pathways enable near-unity quantum efficiency under physiologically relevant fluctuations. These results establish a unified network perspective for understanding energy transport in complex molecular systems and provide general design principles for robust artificial light-harvesting materials.

Physics-Informed Machine Learning for Enzyme Catalysis

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Abstract

The Enzymes are nature's catalysts, driving chemical reactions essential for life. However, understanding how enzymes function at the molecular level remains highly challenging. An enzyme can bind its substrate in multiple configurations and proceed through several reaction pathways, many of which are difficult to capture experimentally. In particular, transition states (TSs), despite being central to understanding reaction mechanisms and kinetics, as well as to the design of transition-state analogue inhibitors, are almost impossible to observe experimentally due to their transient nature. The only viable way to characterize these high-energy TSs is through physics-based computational approaches. However, such methods are often computationally expensive and require detailed, system-specific knowledge that is either unavailable or difficult to obtain. Moreover, they typically identify TSs via static optimization, neglecting the inherently dynamical nature of enzymatic reactions, which can limit their accuracy.

To address these fundamental limitations, I will present a physics-informed machine learning (ML) framework that integrates ML with statistical physics and quantum mechanics. This protocol represents a paradigm shift in computational enzymology, moving away from the traditional focus on a single reaction mechanism and its associated global free-energy pathway. Instead, it adopts a probabilistic view of the entire catalytic landscape of the full enzymatic turnover cycle, encompassing multiple interconnected and competing mechanisms, each proceeding through several pathways governed by thermal fluctuations. This approach requires only the three-dimensional structure of the enzyme-substrate complex as input and enables automated exploration of catalytic mechanisms^[1], dynamic identification of key transition states^[2], and quantitative characterization of the thermodynamics and kinetics of the entire catalytic process^[1-3]. The resulting framework has proven to be fast, accurate, and transferable, making it a promising platform for rational enzyme engineering and drug design.

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Second-Sphere Gating Resolves Spectroscopic Heterogeneity in [NiFe] Hydrogenase

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Abstract

The Ni-L and Ni-R intermediates of [NiFe] hydrogenases exhibit well-documented spectroscopic heterogeneity, the structural origin of which has remained unresolved for decades. Using a multiscale computational approach — combining long-timescale MD, QM/MM calculations, large quantum cluster models, and EPR/IR spectroscopy simulations — we resolve this heterogeneity in *Desulfovibrio vulgaris* Miyazaki F (*DvMF*). We show that the multiple spectroscopic signatures of Ni-L and Ni-R arise from a thermodynamic preference for Glu34 protonation along the Cys546-Glu34 proton-transfer coordinate. This proton-sharing motif is gated by second-sphere residues Thr18 and Arg479, which strongly modulate catalytic-state energetics and govern proton localization. Only Glu34-protonated models quantitatively reproduce experimental EPR *g*-tensors and hyperfine couplings, while Cys546 deprotonation yields characteristic CO/CN red shifts. Computational mutagenesis (T18G, T18D, R479K) directly validates these mechanistic assignments. Results are consistent across O₂-sensitive *DvMF* and O₂-tolerant *E. coli* Hyd-1, suggesting broad conservation of this gating mechanism within Group 1 [NiFe] hydrogenases. These findings reconcile long-standing models of Ni-L/Ni-R heterogeneity and offer design principles for bioinspired hydrogen-evolution catalysts.^[1]

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Beyond Sequence and Shape: DNA Flexibility Governs Transcription Factor Recognition

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Abstract

Precise recognition of short DNA motifs by transcription factors (TFs) is central to gene regulation; however, nucleotide sequence alone does not fully explain why only a subset of the many near-identical genomic motif instances is occupied in vivo. Two major recognition mechanisms are well established: base readout and shape readout. DNA, however, is not static. It can bend, twist, and stretch with sequence-encoded propensities that are not fully captured by either base identity or static DNA shape. This work evaluates intrinsic DNA conformational flexibility as a complementary, interpretable layer of the TF-DNA recognition code.

We developed DNAflexpy, a Python package that encodes five sequence-derived flexibility descriptors representing three modes of deformation: bending, torsional flexibility, and stretching. Flexibility-augmented machine-learning models trained on HT-SELEX and protein-binding microarray datasets consistently improved prediction relative to sequence-only baselines, complemented DNA-shape models across experimental platforms, and identified family-specific flexibility footprints-recurrent hotspots within motifs and flanking regions that correspond to deformations observed in TF-DNA complex structures [1].

We further extended this framework to cooperative TF binding and nucleosomal DNA. Analysis of CAP-SELEX data comprising more than 3,000 affinity tables for 218 TFs indicated that DNA flexibility contributes to cooperative binding. On nucleosomal DNA, models built from 226 TF-nucleosome datasets from NCAP-SELEX suggested that flexibility contributes to pioneer-TF engagement. Together, these analyses support DNA conformational flexibility as an interpretable, sequence-encoded determinant that acts in concert with base and shape readout. By providing both a computational tool and a unifying modelling framework, this work helps rationalize why only a fraction of cognate motifs are productively occupied in vivo and may contribute to improved decoding of cis-regulatory grammar and the design of synthetic regulatory elements.

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RNA recognition beyond structure: insights from disordered protein domains

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Abstract

Association of protein and RNA is crucial for several vital cellular processes like telomere maintenance, translation, splicing and other post-translational processing. RNA binding proteins (RBPs) are a class of proteins with RNA binding domains (RBDs) that can specifically recognize and bind RNA facilitating their downstream processes^[1]. Molecular recognition between RBPs and RNA is the preliminary step, which involves dynamic rearrangements of their structures. RBPs are typically small (~100 residues in length) and the binding sites are mostly disordered loops or regions to facilitate adaptive recognition of their diverse target RNAs. Particularly, the RG/RGG rich domains are interesting in this aspect that they are intrinsically disordered RBPs, as seen in the FET and hnRNP family of proteins. Among the folded RBPs, RNA Recognition Motif (RRM) domain is a commonly occurring RBP specific for single stranded regions of RNA and binds 2-3 nucleotide stretches via hydrogen bonds and stacking interactions. FET and hnRNP family of proteins comprise both these RBDs to facilitate RNA recognition. Interestingly, the FET family proteins also possesses a ZnF domain that specifically recognizes single stranded RNA. We have modeled the interaction of FUS and hnRNP A1 with their substrate RNAs, a stem-loop RNA, a single stranded RNA and telomeric RNA G-Quadruplexes using computational methods. Through our work, we have provided a molecular picture of protein-RNA recognition and identified the key sequence as well as structural features of FUS and hnRNP A1 responsible for binding with their substrate RNA. The interplay of several RBDs and the non-specific interaction of RGG domain in FUS improves RNA affinity, while the same induces GQ instability in case of hnRNP A1, highlighting that IDPs can involve in specific functions facilitated by their dynamic recognition.^[2, 3]

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High-Dimensional Free Energy Surfaces of Chemical Reactions

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Abstract

Biased molecular dynamics methods are widely used to accelerate transitions between metastable states and for computing the underlying free energy landscapes. The computational efficiency of biased-sampling methods decreases with increasing dimensionality of the space to be sampled, limiting their predictive power. High-entropy states often lead to poor exploration and degrade accuracy. We proposed a family of methods called “Sliced Sampling” to overcome these limitations. Sliced Sampling methods allow for controlled exploration and efficient computation of high-dimensional free-energy landscapes. Moreover, many collective variables can be biased simultaneously. Sliced sampling methods enable accurate calculation of free energy barriers and reaction rate constants. In this presentation, I will discuss recent developments and applications of Sliced Sampling methods in the study of complex chemical reactions.

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Fluctuation-Governed Molecular Dynamics: From Water Anomalies to Mass-Selective Transport

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Abstract

Molecular motion in condensed phases is often governed not only by average structures or static free-energy landscapes, but also by fluctuations that modulate the relevant pathways in time. I will first briefly introduce our studies of supercooled water, in which thermodynamic anomalies are closely related to fluctuations between locally distinct hydrogen-bond network structures.[1-3] By analyzing molecular jump dynamics, we have developed a dynamic-disorder framework that identifies slow variables controlling intermittent barrier-crossing events and clarifies how these variables grow in spatial extent as dynamics slow.[4-6] This framework has also been applied to other transport problems; for example, it has provided insight into Li⁺ conduction mechanisms in glassy solid-state electrolytes and tracer particle diffusion in fluctuating environments.[7-9] I will then discuss mass-selective diffusion in dynamic nanopores of soft porous crystals, a class of flexible metal–organic frameworks. We modeled molecular transport as Brownian motion on a fluctuating periodic energy landscape, in which energy barriers switch between open and closed states due to local gating motions. This model reveals that diffusivity can be maximized at an optimal energy-fluctuation rate and that this optimal rate depends on the molecular mass. As a result, small mass differences, such as those between H₂O and D₂O, can be amplified into large differences in diffusivity.[10]

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Efficient finite-element methods for fast *ab initio* calculations with meta-GGA functionals

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Abstract

First-principles modelling has become an indispensable tool for predicting and understanding material properties across a wide range of applications, with Kohn–Sham density functional theory (DFT) serving as the workhorse of electronic-structure calculations. Although Kohn–Sham DFT is formally exact, the exchange–correlation energy must be approximated, leading to a hierarchy of density functional approximations with increasing levels of complexity and accuracy. Kinetic-energy-density-dependent meta-generalized gradient approximation (τ -mGGA) functionals, such as SCAN and its regularized and restored variant r2SCAN, incorporate the kinetic energy density in addition to the local electron density and its gradient, offering improved accuracy at the expense of greater computational and numerical complexity.

In this talk, we present finite-element-based methods for τ -mGGA functionals that enable efficient and scalable electronic-structure calculations for systems containing tens of thousands of electrons. The finite-element formulation proposed, incurs the same computational cost per iteration as traditionally used GGA functionals, in contrast to conventional plane-wave DFT approaches, where τ -mGGA calculations can be 3–5 $\times$ more expensive per iteration than GGA calculations. Despite their improved accuracy, τ -mGGA functionals can suffer from numerical instabilities and slow convergence of self-consistent field (SCF) iterations in DFT. To address this challenge, we develop a preconditioned density-mixing scheme within the finite-element framework that accelerates SCF convergence by leveraging a low-rank approximation of the dielectric matrix. These developments enable accurate and scalable quantum-mechanical simulations of complex material systems while improving the computational efficiency of advanced local density functional approximations. This ability to rapidly generate high-fidelity first-principles data at scale provides a powerful pathway for training more accurate machine-learning models for accelerated materials discovery and prediction.

STEM: A Dynamic Electrostatic Simulation Model for Ion-Coordinated RNA Folding

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Abstract

RNA folding into functional tertiary structures is critically influenced by its surrounding ionic atmosphere, which screens the long-range electrostatic repulsion between negatively charged phosphate groups. While monovalent ions primarily stabilize secondary structures, divalent magnesium (Mg^{2+}) ions promote tertiary folding through dynamic transitions between outer-sphere and inner-sphere coordination with the phosphate backbone.^[1] Existing RNA structure prediction methods largely rely on static contact maps and therefore fail to capture the dynamic ion-coordination states that regulate conformational transitions and folding pathways. Here, we present the Structural Topology-Based Electrostatics Model (STEM), a multiscale hybrid framework that explicitly describes the dynamic exchange between outer-sphere and inner-sphere Mg^{2+} coordination while treating monovalent ions implicitly through the Generalized Manning Counter-ion Condensation Theory.^[2,3] We validate STEM on structurally diverse RNA systems by accurately reproducing crystallographic Mg^{2+} binding sites, experimental preferential ion-interaction coefficients, and SAXS-derived radii of gyration. Application to a 58-nucleotide rRNA domain reveals that the formation of a chelated Mg^{2+} -mediated tertiary contact drives the final transition from an intermediate to the native state and regulates the molecule's conformational breathing. These results demonstrate that RNA folding is governed not only by native structural contacts but also by the dynamic exchange between distinct Mg^{2+} coordination states that mediates long-range RNA contacts. By moving beyond static contact-map descriptions, STEM provides a physically grounded and computationally efficient framework for investigating RNA folding dynamics, ion-dependent free-energy landscapes, and the mechanisms underlying RNA structure and function across varying salt conditions.^[4]

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Development of an automatic differentiation-based force-field optimization library for organic electrolytes

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Introduction

Lithium-ion batteries typically employ liquid electrolytes consisting of lithium salts dissolved in organic solvents, and molecular crystal electrolytes have also recently attracted attention [1]. Classical molecular dynamics (MD) is a powerful tool for studying ion transport; however, its application is limited by force-field accuracy. For instance, standard force fields such as GAFF and OPLS fail to reproduce dynamic properties of sulfolane, a widely studied solvent (SL; Fig. 1a) [2]. To address this issue, we develop iMolCRAFT (Ionic Molecular Crystal Automatic Force-field Tool), a framework that exploits automatic differentiation [3] to optimize force fields, and we demonstrate its efficiency on SL-based liquid and crystalline systems.

Computational details

The initial force field was constructed using GAFF2 with RESP charges, and the parameters were subsequently optimized. The loss function was defined based on structural properties obtained via PBE-D3 level universal machine learning interatomic potential (uMLIP)-MD [4]. Gradients of the loss with respect to force-field parameters were evaluated using thermodynamic perturbation theory. As reference data, radial distribution functions (RDFs), density, and cell parameters were employed.

Results and discussion

We first evaluated the self-diffusion coefficient of pure SL using the original GAFF. The calculated value ($0.86 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$) markedly underestimated the experimental value extrapolated to zero concentration ($14.7 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$) by a factor of ~ 17 . Comparison between GAFF and uMLIP-MD RDFs (Figs. 1b) revealed discrepancies in both the onset position and height of the first O–H correlation. The optimized force field improves agreement with RDFs of MLIP-MD. Consequently, the self-diffusion coefficient increases to $20.1 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$, in good agreement with experiment. The viscosity is also reproduced, yielding $6.1 \pm 1.5 \text{ mPa} \cdot \text{s}$ compared to the experimental value of $10.23 \text{ mPa} \cdot \text{s}$. We then applied the same optimization strategy to the crystalline phase (LiBF₄SL; Fig 1c), which resulted in agreement for both RDFs (Fig. 1d) and lattice parameters ($L_a=5.16 \text{ \AA}$, $L_b=9.06 \text{ \AA}$, $L_c=18.41 \text{ \AA}$; experiment: $5.16, 8.85, 18.34 \text{ \AA}$), thereby demonstrating that the refined force field can accurately reproduce the crystal structure.

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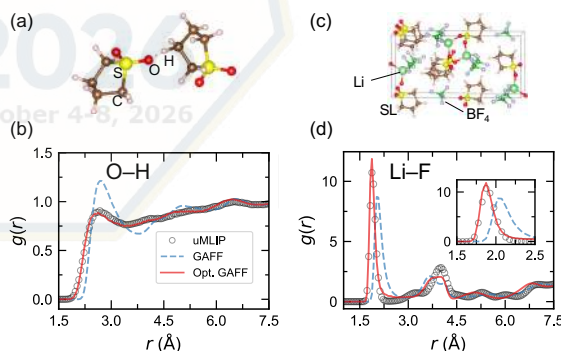


Fig. 1 (a) Association structure of sulfolane (SL) and (b) O–H radial distribution function (RDF) of in the liquid phase. (c) Unit cell and Li–F RDF of LiBF₄SL crystal.

2-Dimensional Binary Crystals in Additive Hard Disk Mixtures

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Abstract

The hard disk model is a foundational system for understanding two-dimensional phase behavior. Its extension to binary mixtures introduces additional structural complexity and kinetic constraints that hinder the formation of ordered phases. Although geometric constructions predict a variety of binary crystals at high densities, these phases often fail to self-assemble in simulations due to slow dynamics and competing phase separation. Recently, we have shown the spontaneous formation of the H₂ hexagonal binary hard disk crystal in additive mixtures using event-driven molecular dynamics [1]. We show that crystallization is highly sensitive to thermodynamic conditions, requires long equilibration, and is facilitated by particle swap moves. Despite its high packing fraction, the H₂ crystal forms spontaneously at equimolar composition and near-ideal size ratio but is kinetically hindered at intermediate densities by the formation of competing one-component hexagonal phases. Our results identify the conditions under which H₂ binary crystals spontaneously form and show that their emergence can proceed through non-classical nucleation pathways involving metastable intermediates. We extend this work to find other 2-dimensional binary hard disk crystals predicted using geometric construction [2] and infinite pressure phase diagram for non-additive hard disk mixtures [3]. Our simulation results show that advanced simulation techniques such as using particle swap moves and increasing small particle concentration facilitate formation of complex crystal structures.

Keywords: Computational/Numerical; Theoretical (physics)

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Affinities of Polymers to Water Studied by All-Atom MD Simulation and a Solvation Theory

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The affinity to water is a key property of a polymer in academic and industrial uses. It reflects sensitively the intermolecular interaction between water and the polymer as well as the mode of aggregation of the polymer medium (crystalline vs amorphous, for example). The atomic-level description is thus necessary for elucidating the interactions of a polymer with water, and all-atom molecular dynamics (MD) simulation is a method for meeting this necessity. In the present work, we analyze the dissolution of water into a variety of homo- and copolymers in their bulk states and the work of adhesion corresponding to formation of polymer-water interfaces, by combining all-atom MD and a statistical-mechanical theory of solvation.

The extent of water dissolution is determined by the dissolution free energy of the water molecule into a polymer medium of interest. We compute the free energy of water dissolution efficiently by employing the energy-representation theory of solvation. This theory expresses the solvation free energy as an approximate functional of distribution functions of the solute-solvent pair energy, and the free energy of water dissolution is calculated as a solvation free energy by viewing water as the solute and the polymer as the solvent. Since structural information is projected out in the energy-representation formalism, the applications are straightforward to systems involving flexible molecular species such as polymer, lipid, and surfactant. The distribution functions are to be constructed only in the pure polymer system without the water solute and the water-polymer system with fully coupled solute-solvent interaction. Use of the energy-representation method reduces the computational load of free energy since intermediate states adopted in standard free-energy methods such as free-energy perturbation and thermodynamic integration are not employed. It is demonstrated that all-atom treatment is predictive for the free energy of water dissolution, irrespective of the hydrophobicity and hydrophilicity of the homopolymer. The free energy of water dissolution is further examined in copolymers of ethylene and component compounds with varied hydrophilicity. It is found that the dissolution free energy of water is not affected by the overall topology of the copolymer (periodic vs block) and that the hydrophobicity of the copolymer is enhanced when the hydrophobic and hydrophilic components are shorter and are bonded along the chain in fragmented manners.

The work of adhesion between liquid water and a solid polymer is also computed by all-atom MD combined with the energy-representation theory of solvation. In this case, the whole solid of the polymer is treated as the solute and the adhesion work is formulated as the free energy of solvation of the polymer solid in solvent water. The solute-solvent interaction is then operative across the water-polymer interface. The energy-representation method can still be employed for a “solvation” in an inhomogeneous medium since it provides the free energy only through statistics of the solute-solvent energy without referring to structural information. It is demonstrated that the adhesion works computed approximately by the energy-representation method agree well with the exact values. The water-polymer interactions that are responsible for the strength of adhesion is further addressed within the framework of the solvation theory.

Threading and Stress Overshoot in Ring-Linear Polymer Blends under Elongational Flows

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Abstract

Ring polymers blended with linear chains exhibit strongly nonlinear rheology under elongational flow because linear chains can thread through the rings and form transient topological constraints. Using coarse-grained molecular dynamics simulations based on the Kremer–Grest model, combined with the SLLOD equations of motion under generalized Kraynik–Reinelt boundary conditions for large-strain elongation, we have clarified the topological origin of stress overshoot in such blends across three complementary settings.

First, for ring–linear blends under *biaxial* elongation, we reported the first observation of a viscosity overshoot in this geometry, most pronounced in weakly entangled melts.^[1] The overshoot arises from cooperative ring–linear dynamics: linear chains penetrating a ring stretch it within the elongational plane, and the subsequent release of these chains lets the ring recoil. The threshold strain rate separating linear and nonlinear response scales as $\dot{\epsilon}_{\text{th}} \sim N_L^{-1/2}$, deviating from the N_L^{-2} expected from the Rouse relaxation time.

Second, for *multicyclic*/linear blends under biaxial elongation, the overshoot is steeper than in the monocyclic case and is driven by a distinct mechanism.^[2] A topological transition, in which a ring changes from an open to a closed double-folded state, sharply reduces the ring stress. We showed that structural symmetry of the rings within a multicyclic chain is indispensable for the overshoot: asymmetric chains undergo the same transition but show no overshoot.

Third, for ring–linear blends under *uniaxial* elongation, we identified a threshold chain length for the overshoot.^[3] Equi-weight flexible blends show monotonic stress growth for short chains ($Z \leq 2$) but a clear overshoot once the entanglement number reaches $Z \approx 4$. Gauss-linking-number analysis reveals that each ring is then multiply threaded by several linear chains, and the rapid release of these constraints—a thread-to-unthread transition driven by the ring component—produces the peak. We further predict the associated 2D small-angle neutron scattering patterns as a route to experimental validation.

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Exploring the conformational landscapes of polyampholytes and disordered proteins with minimalist models

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Unlike folded proteins, intrinsically disordered proteins (IDPs) lack a well-defined three-dimensional structure, challenging the conventional structure–function paradigm. Their sequences typically contain a few hydrophobic residues and an abundance of charged and polar amino acids, making them analogous to polyampholytes with tunable flexibility. Using the venerable Kremer–Grest model, we demonstrate that the interplay between charge patterning and bending rigidity dictates the equilibrium structures of polyampholytes, often giving rise to exotic morphologies. We also show the emergence of sluggish dynamics and ergodicity breaking for very stiff chains. Furthermore, employing various minimalist models, we investigate the conformational dynamics of the LAF1 sequence and its shuffled variants, and show that their energy landscapes encode distinct structural features, which could play a critical role in phase separation.



From bulk solution to biological membranes: Molecular dynamics investigations of the behavior of biosurfactants

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Abstract

Biosurfactants exhibit a wide range of biological and physicochemical activities that are governed by their self-assembly behavior and interactions with biological membranes. Using molecular dynamics simulations, we investigate how molecular architecture influences self-assembly and membrane activity in biosurfactant systems. For surfactin, increasing hydrocarbon chain length promotes the formation of larger, more spherical aggregates and alters hydrogen-bonding patterns within the peptide ring. Surfactin–membrane interactions further reveal that membrane susceptibility depends strongly on lipid chemistry, with ester-linked and tetraether lipid membranes exhibiting greater perturbation than diether systems. In oligomeric imine-bond biosurfactants, increasing oligomerization leads to smaller aggregation numbers and a transition from spherical micelles to interconnected assemblies. Free-energy calculations reveal that aggregate size and surfactant architecture strongly influence monomer exchange dynamics, providing a mechanistic explanation for their experimentally observed antimold activity. Together, these results demonstrate how biosurfactant molecular architecture governs self-assembly, aggregate stability, and membrane interactions, providing molecular-level design principles for biosurfactants with tailored biological and physicochemical properties.

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Large-Scale Molecular Dynamics Study of Gas Effects on Water Droplet Splashing

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Recent experimental studies have shown that droplet splashing strongly depends on the surrounding gas pressure. When a liquid drop impacts on a solid surface, a thin lamella spreads radially and may lift off from the substrate, producing secondary droplets. Xu et al.^[1] demonstrated that reducing the ambient pressure suppresses splashing. Riboux and Gordillo^[2] subsequently proposed a theoretical model in which aerodynamic lift generated by the surrounding gas governs splash formation.

Molecular dynamics (MD) simulations have recently been applied to nanodroplet impacts, revealing nanoscale phenomena such as internal film rupture, finger formation, and hole generation in the spreading lamella^[3,4]. However, previous simulations were limited to droplets with diameters of about 10 nm, making it difficult to reproduce experimentally observed splash dynamics on smooth solid surfaces.

In this study, large-scale MD simulations were performed using the SPC/E water model. The simulated droplet consisted of five million water molecules with an initial diameter of approximately 67 nm. To investigate gas effects, argon molecules were introduced into the system, and the gas pressure was varied from 5 to 20 MPa. Simulations were carried out on smooth solid surfaces with different wettabilities.

The results show that increasing the gas pressure promotes lift-off of the spreading lamella. Under sufficiently high pressures, the liquid sheet develops into a crown- or corona-like structure, and secondary droplets are ejected from its rim. These behaviors are qualitatively consistent with experimental observations. The present study demonstrates that sufficiently large atomistic simulations can reproduce realistic droplet splashing and provide a useful approach for investigating gas-liquid interactions during high-speed droplet impact.

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Fragility-Dependent Structural Bottlenecks in Jump Dynamics of Supercooled Glass Formers

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Abstract

Fragility characterizes how rapidly a glass-forming liquid slows down upon supercooling, but whether strong and fragile behavior arise from the same microscopic relaxation mechanism remains unclear. Recent studies of supercooled water^[1], silica^[2], and the Kob–Andersen Lennard-Jones liquid^[3] have shown that slowly evolving local structural variables modulate microscopic jump rates and give rise to dynamic disorder. However, how the nature and spatial extent of these rate-controlling structural variables change with fragility remain unresolved. Here, we address this question using a density-tunable soft-repulsive binary mixture spanning distinct fragility regimes and analyze particle jump dynamics within the framework of dynamic disorder. Across these regimes, we show that increasing fragility leads to progressively broader cage-lifetime distributions and increasingly non-exponential survival probabilities, revealing non-Poisson cage-to-jump statistics governed by fluctuating jump rates and slowly evolving structural variables. To characterize their structural origin, we first identify the neighbor ranks most strongly coupled to jump motion using Kullback–Leibler (KL) divergence and Pearson correlation analyses. We then introduce a structural slowness parameter (SSP) that combines these neighbor-distance fluctuations into a reduced slow coordinate for constructing the slow-fluctuation survival probability. Comparison with the actual survival probability shows that localized neighbor-distance fluctuations control the jump rate in the strong-like regime, whereas extended neighbor rearrangements become relevant in the intermediate and fragile regimes, increasing the effective dimensionality of the slow-variable space. In the fragile regime, distance-based descriptors become insufficient at the lowest temperature, where Voronoi free volume captures additional cage-volume fluctuations in the rate-controlling slow variable. Point-to-set correlations grow with fragility, but the spatial extent of the slow variables exceeds the point-to-set length. These results show that fragility changes the structural bottleneck for microscopic rate fluctuations, linking dynamic disorder, multidimensional slow variables, and static correlations in glass-forming liquids.

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Designing High-Performance Energy Storage Systems for Decarbonization

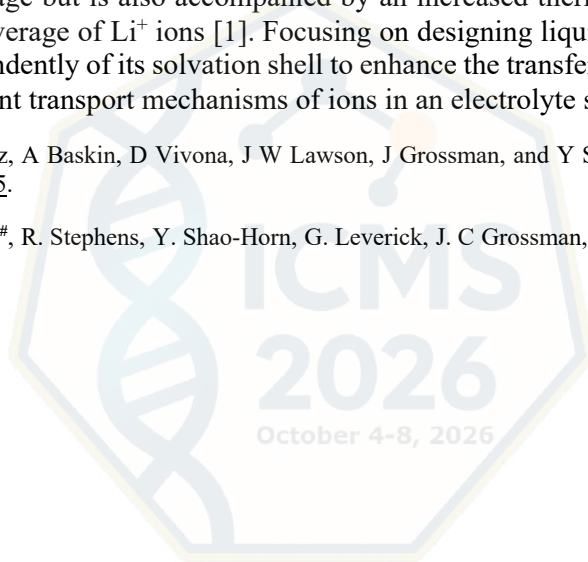
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There is an urgent need to reduce our global carbon dioxide emissions to mitigate climate change. While low-cost electricity from solar and wind sources provides exciting opportunities to reduce emissions, the transition to decarbonization is only possible once energy storage devices with higher energy densities, longer lifespans, and faster charging capabilities are available. In this seminar, I will present a computational approach to establishing design guidelines for high-performance energy storage devices. I will discuss the driving forces and thermodynamic barriers of Li^+ ion adsorption onto commercial electrode materials in different salt electrolytes using insights from state-of-the-art computational techniques, like molecular dynamics (MD), machine learning (ML), and density functional theory (DFT) simulations. I will show that the weaker cation-anion pairing enhances the driving force for adsorption for an electrode-electrolyte interface with zero cation coverage but is also accompanied by an increased thermodynamic barrier at an equilibrium surface coverage of Li^+ ions [1]. Focusing on designing liquid electrolytes where the Li^+ ion diffuses independently of its solvation shell to enhance the transference number, I will also elaborate on the different transport mechanisms of ions in an electrolyte solution [2].

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Electrical conductivity of ionic-liquid based electrolyte for sodium-ion battery development: the effects of cation moieties.

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Abstract

Sodium-ion battery (NIB) is a promising technology for large-scale electrical energy storage systems owing to the low cost and widespread availability of sodium. The safety and performance of NIB can be further enhanced using an ionic liquid (IL) as its electrolyte, whose unique properties include low flammability, a wide liquid-temperature range, and a broad electrochemical window. Known as a "designer solvent", IL can have its properties tailored through structural modification, such as the addition of various moieties. In this work, the iterative combination of MD and density functional theory is employed to investigate the effects of hydroxy, alkoxy, and alkyl moieties attached to IL's cation in altering the electrical conductivity of ternary ionic systems, denoted as [X, Na][FSA], which are relevant to NIB electrolytes. Since the overall transport properties are influenced by the cation-anion coordination, the presence of a cation that can compete with the FSA anion to bind Na is observed to highlight two opposing effects: the weakening of Na-FSA binding that increases the sodium ion transference number, and the increase in viscosity that hampers the overall transport.

Towards Ion Transport Prediction in Battery Materials via MD and Non-Equilibrium MD

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Introduction: Control of ion transport in battery is still of great importance from both fundamental and industrial viewpoints. For conventional Li-ion battery (LIB), (A) concentrated organic liquid electrolyte has attracted much attention owing to its electrochemical stability, while estimation of the ion diffusivity in the electrolyte is still under debate because of possible change of diffusion regime (vehicle vs hopping). In next-generation all-solid-state-batteries (ASSBs), (B) ion-ion correlation and ion-framework coupling in solid electrolyte (SE) have been recent important subjects toward superionic conductors. (C) Regarding electrodes, mixed ionic-electronic conductors (MIEC), ion-electron correlation is so crucial. To give atomistic insights to these questions, we have carried out MD samplings at the levels of density-functional-theory (DFT), machine-learning interatomic potential (MLIP), and conventional force field (FF). Furthermore, we have extended non-equilibrium MD (NEMD) to speed up the calculations of correlated ionic conductivity.

Computational: We calculated ion diffusivity via mean-squared displacement or time-correlation function sampled with MD. DFT-MD calculations were performed using VASP and CP2K codes where PBE functionals with vdW or Hubbard U scheme. Besides, GAFF FF and fine-tuned MACE MLIP were used with LAMMPS and GROMACS codes. Our extended NEMD was implemented to CP2K.

Results and discussion: First we discuss the methodology of NEMD based on the Onsager theory. In addition to the constant field scheme, we have developed constant current scheme using Lagrange multiplier, which significantly accelerates the "correlated ionic conductivity" in sulfide and oxide SEs with reasonable accuracy^[1,2].

Regarding the ion transport in electrode (MIEC), we examined LiCoO₂ and LiNiO₂, representative cathode materials for LIB, and showed dominance of electronic conductivity for the performance^[3]. We also investigated several Prussian blue analogues (A_xM[M'(CN)₆]: A=Alkaline atom, M & M'=transition metal) for Na-ion battery (NIB) cathode and demonstrated that the dynamical framework distortion enhances the Na-ion transport^[4,5]. On the other hand, calculated Na-ion self-diffusivity in hard carbon, a major NIB anode, is found much lower than the experimental values in both DFT-MD and MLIP-MD samplings^[6,7].

Recently, we also studied dependence of Stokes-Einstein relation on the Li-salt concentration in LIBs and suggested novel understanding of parameters in the S-E relation^[8].

These results will provide a more precise understanding of ion transport in battery materials, leading to a more useful guide to control it.

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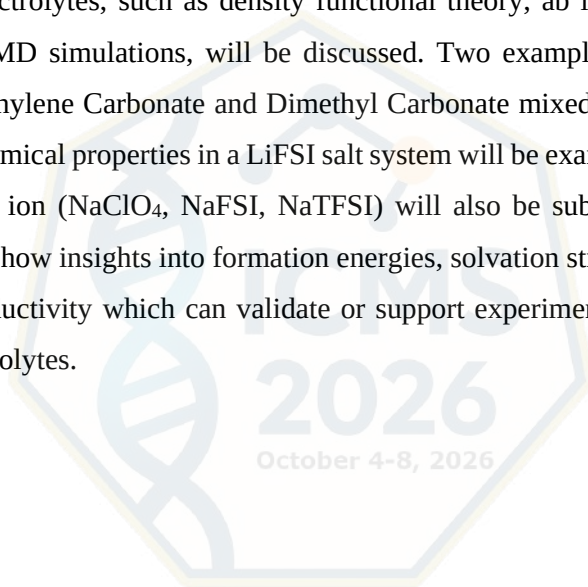
Investigating battery electrolytes: What insights can Quantum Chemistry and (ab initio) Molecular Dynamics simulations offer?

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Carbonate-based lithium battery and sodium battery electrolytes show excellent chemical stability and electrochemical performance. The various computational techniques that are used to study properties of battery electrolytes, such as density functional theory, ab initio molecular dynamics (AIMD), and classical MD simulations, will be discussed. Two examples of electrolytes will be chosen. The effect of Ethylene Carbonate and Dimethyl Carbonate mixed solvent and temperature, on the structure and dynamical properties in a LiFSI salt system will be examined. The effect of anion with a common sodium ion (NaClO_4 , NaFSI, NaTFSI) will also be subsequently discussed. The computational methods show insights into formation energies, solvation structure, ion-pair lifetimes, diffusion and ionic conductivity which can validate or support experimental findings and assist in synthesis of newer electrolytes.



Resolving 10- μ s Li⁺ Hopping Dynamics in Deeply Supercooled Polymer-in-Salt Electrolytes by Molecular Dynamics Simulation

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Solvent-free lithium electrolytes in deeply supercooled states can exhibit near-unity Li-ion transference numbers under anion-blocking conditions, yet the molecular origin of this unusual transport remains difficult to access experimentally.¹ Here, we use long, statistically replicated molecular dynamics simulations extending beyond 10 μ s, together with force fields developed specifically for this system, to resolve the extremely slow ion dynamics of deeply supercooled Li(fluorosulfonyl)(trifluorosulfonyl)imide (Li[FTFSI]) and a poly(methyl methacrylate) (PMMA)/Li[FTFSI] polymer-in-salt electrolyte at 360 K. The long simulation times are essential for obtaining converged ion-ion cross-correlations and for directly characterizing rare, intermittent Li⁺ hopping events in the supercooled regime. Ionic conductivities calculated using full correlated-ion dynamics closely reproduce the available experimental values for both neat Li[FTFSI] and the PMMA-containing electrolyte.

In the deeply supercooled state, Li⁺ diffuses about an order of magnitude faster than FTFSI⁻, leading to a near-unity transference number. Molecular-level analysis reveals that Li⁺ transport occurs through intermittent hopping between coordination environments, whereas FTFSI⁻ motion is largely restricted to rotational and vibrational relaxation. The hopping mechanism is confirmed by time-dependent pair correlation functions, which capture the slow decorrelation of Li⁺ local structure over microsecond timescales. Incorporating PMMA introduces pronounced spatial heterogeneity: Li⁺ dynamics are suppressed near polymer-rich regions but enhanced in polymer-dilute domains, where modified local coordination facilitates hopping. Although most hopping events are isolated, a significant fraction involves cooperative local rearrangements. Cross-correlation analysis further reveals weak cation-anion coupling relative to highly concentrated liquid electrolytes, which helps explain why Li⁺ remains the dominant charge carrier.

These simulations provide a microscopic basis for the anomalously high Li-ion transference in solvent-free, deeply supercooled electrolytes and demonstrate how long-timescale molecular simulations can reveal transport mechanisms otherwise obscured by extremely slow dynamics. Polymer-stabilized supercooled electrolytes therefore emerge as promising candidates for next-generation high-transference-number Li-ion conductors.

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Electronic Structure and Charge Storage Mechanisms in Perovskite/MXene Heterostructures: A First-Principles Study

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Abstract

Supercapacitors are promising due to their high power density and long cycle life.[1] However, their performance largely depends on the electrode's electronic structure, particularly the Fermi-level density of states (DOS), which directly governs the quantum capacitance (CQ), the theoretical limit of capacitive performance [2]. We aim to search for high-performance electrodes for supercapacitors and identify highly efficient energy storage materials. New materials, such as halide perovskites, are tested for their properties as highly capacitive electrodes that can be charged very quickly and retain their capacitance over long periods of time. We investigated conductive 2D sheets of MXenes, which have superior electrochemical properties and, for the first time, a spin-polarized density functional theory calculation of the halide perovskite KNiF₃ as well as a composite material of KNiF₃ perovskite and Ti₃C₂T_x MXene sheets. The critical parameter for the assessment of the quantum capacitance (CQ) of an electrode, the Fermi-level density of states (DOS), as well as the work function of the investigated materials, were calculated. We found the DOS at the Fermi level of the semiconducting KNiF₃ to be negligible with Ni-3d and F-2p hybridized states being the dominant contributions. Consequently, the calculated CQ(EF) of 40.9 $\mu\text{F cm}^{-2}$ is very low. In marked contrast, the metallic Ti₃C₂T_x MXene shows a very high DOS at the Fermi level, which is mainly composed of Ti-3d states, resulting in a high CQ(EF) of 224.9 $\mu\text{F cm}^{-2}$, which is more than 5 times higher than that of KNiF₃. The interfacial charge transfer between the perovskite and the 2D MXene sheets in the KNiF₃/Ti₃C₂T_x composite material results in a substantially modified electronic structure close to the Fermi level, i.e. a high DOS at the Fermi level and thus a high CQ(EF) of 209.7 $\mu\text{F cm}^{-2}$, which is approximately 5.1 times higher than that of KNiF₃ perovskite. A plot of the CQ versus gate voltage reveals that the KNiF₃/Ti₃C₂T_x composite material has a wider potential window of high capacitance than that of the pristine KNiF₃ perovskite. Thus, the KNiF₃/Ti₃C₂T_x composite material offers advantages for supercapacitor applications. The findings can be utilized to elucidate atomic-scale charge storage mechanisms and to design hybrid perovskite-MXene electrode experiments.

Key Words: DFT, Halide Perovskites, Supercapacitors, Density of state, Quantum capacitance

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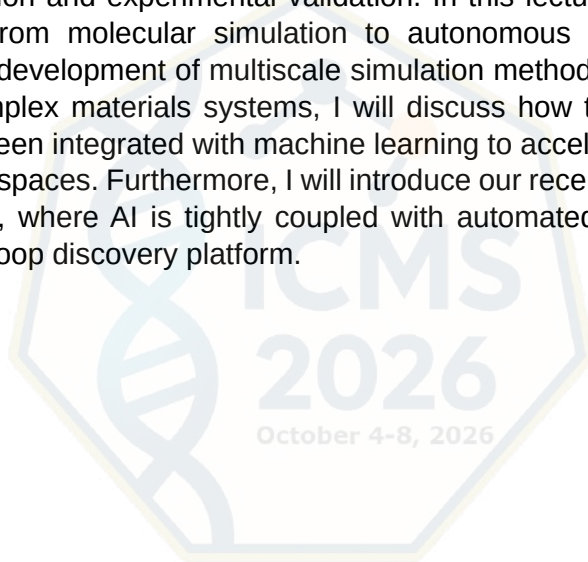
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From Molecular Simulation to Autonomous Materials Discovery

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Over the past two decades, molecular simulation has become an indispensable tool for understanding and designing functional materials across multiple length and time scales. Physics-based computational methods, including density functional theory, molecular dynamics, and reactive force fields, have significantly advanced our ability to predict materials properties and elucidate reaction mechanisms. However, despite these achievements, the conventional simulation-driven discovery paradigm remains fundamentally limited by the vastness of chemical space and the iterative nature of hypothesis generation and experimental validation. In this lecture, I will present our research journey from molecular simulation to autonomous materials discovery. Beginning with the development of multiscale simulation methodologies and reactive force fields for complex materials systems, I will discuss how these physics-based approaches have been integrated with machine learning to accelerate the exploration of materials design spaces. Furthermore, I will introduce our recent efforts toward self-driving laboratories, where AI is tightly coupled with automated experimentation to establish a closed-loop discovery platform.



Molecular matchmaking: Identifying the molecular determinants of G protein selectivity in GPCRs

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Abstract

G protein-coupled receptors (GPCRs) are master regulators of cell signaling that function by coupling with G protein transducers. Despite sharing similar structural architectures, these receptors exhibit remarkable selectivity and varying affinities across a diverse family of G protein sub-types^[1]. Misregulation of the GPCR-G protein molecular interactions are linked to numerous human diseases, making the underlying rules of selectivity a central challenge in structural biology and pharmacology. In this talk, we focus on the β_1 -adrenergic receptor that regulates cardiac function and has only recently been shown to exhibit multi-subtype coupling. To identify the molecular determinants of subtype-specificity, we use a hybrid approach combining molecular dynamics simulations at multiple resolutions (atomistic and coarse-grained) with machine learning classification algorithms. Our simulations successfully validate the core receptor-G protein interactions previously mapped by structural biology, and highlight the remarkably invariance of the core protein-protein contacts for different G protein subtypes. Surprisingly, we show that the primary selectivity filter is located outside this core interface, arising instead from the intrinsically disordered loop domains. We identify differential intracellular and C-terminal loop domain engagements that allosterically modulate the protein-protein interactions. Interestingly, we highlight an important role of lipids, demonstrating that the nano-environment of the receptor is uniquely modulated by each G protein sub-type. In particular the charged lipids, such as phosphoinositides (PIPs), distinguish G protein sub-types and contribute to coupling selectivity. Overall, by resolving these complex biological communication networks, we demonstrate that selectivity is not dictated by static protein-protein contacts. Instead, our work highlights a dynamic network and protein-protein and protein-lipid interplay, offering fresh perspectives on how proteins process information while providing a structural blueprint for designing personalized, next-generation therapeutics.

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Twisted Energy Landscapes: Multiscale Simulations Reveal Geometry-Controlled Amyloid- β Diffusion at Heterogeneous Interfaces

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Abstract

The dynamics of amyloid- β (A β) at heterogeneous interfaces play a central role in molecular recognition and fibril growth, yet the underlying physical mechanisms remain poorly understood. In this presentation, I will introduce a multiscale simulation framework that integrates coarse-grained molecular dynamics, atomistic simulations, and free-energy analysis to investigate how interfacial geometry governs A β dynamics across multiple spatial scales. Coarse-grained simulations reveal that A β monomer diffusion on fibril surfaces deviates from classical Brownian motion and is instead dictated by anisotropic, periodically modulated free-energy landscapes imposed by fibril architecture. Rather than serving as passive substrates, fibril surfaces encode preferred diffusion pathways and kinetic barriers through their structural geometry. This geometry-dependent energy landscape provides a physical mechanism for regulating monomer transport during fibril elongation. Building upon these mesoscale observations, atomistic simulations further demonstrate how hydration structure and chemical heterogeneity reshape interfacial free-energy landscapes. Analyses of solvent organization reveal that hydration water actively mediates protein-surface interactions, while simulations of A β 42 binding to ganglioside GM1 show that receptor organization selectively stabilizes distinct binding conformations through cooperative structural effects. Together, these results establish a unified multiscale picture in which interfacial geometry, hydration, and chemical specificity collectively determine the free-energy landscapes governing A β diffusion and molecular recognition. This work highlights how molecular simulations can bridge dynamic behavior across length scales and provide mechanistic insight into protein aggregation at biologically relevant interfaces.

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Molecular dynamics of membrane peptide binding and assembly for rational sequence design

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Abstract

The rational and *de novo* design of membrane peptides and proteins remains a major challenge despite significant advancements in the field of protein design. Current design strategies have largely focused on the thermodynamic stability of the target structure, whereas the transient states associated with membrane insertion, oligomerisation, and structural rearrangement have not been comprehensively addressed.^[1] Particularly in membrane systems, understanding how a given sequence reaches the intended structure is relevant both to predicting experimental tractability and to avoiding unintended metastable states. From this perspective, we examine membrane binding and assembly of natural and designed peptides primarily through molecular dynamics simulations.

First, building on our recent success in *de novo*-designed peptide-based channels,^[2] we analyse the molecular interactions associated with membrane insertion, oligomeric intermediates, and the emergence of dynamic channel assemblies, in response to an external electric field.^[3] Secondly, for peptides originating from intrinsically disordered regions (IDRs) of proteins, we characterise the interactions between the peptides and the membrane surface in relation to the lipid compositions.

These simulations indicate that charged residues flanking the membrane-spanning segment, membrane potential, lipid composition, and local interactions at the water–membrane interface may impact the design outcomes. These findings will offer a molecular framework to enhance the success rate of membrane peptide and protein design and facilitate the engineering of more dynamic membrane-associated functions.

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Unraveling Molecular Interactions Responsible for Microtubule-Wetting by Biomolecular Condensates

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Abstract

Microtubule-condensate interactions play a central role in regulating cytoskeletal processes such as cell division, vesicle transport, intracellular organization, and cellular motility [1,2]. Through selective recruitment of biomolecules, condensates can modulate microtubule dynamics, organization, and function [2,3]. However, the molecular principles governing condensate binding to microtubules remain poorly understood. The large size and structural complexity of microtubules, combined with the slow relaxation and heterogeneous nature of biomolecular condensates, make systematic molecular-level investigations computationally challenging.

By integrating coarse-grained molecular simulations with sequence-pattern analysis, we unravel the sequence features that promote stable condensate-microtubule interactions. Our investigation reveals the nature of the predominant interaction motifs that drive microtubule binding: positively charged hydrophobic “blocks” [4]. These motifs facilitate binding through complementary electrostatic and hydrophobic interactions with the microtubule surface. We also identified the preferential interaction regions on the microtubule surface and showed that the predicted binding hotspots are consistent with available experimental observations. Together, these findings pave the way for establishing the molecular grammar for condensate-microtubule recognition and developing a predictive framework for understanding, designing, and screening IDP sequences with targeted microtubule-binding properties.

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Preservative kinetics and influence of surfactants on Gram-negative bacterial membrane partitioning

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Abstract

Preservatives are primarily used for their antimicrobial properties and form an important component of food, cosmetic and drug formulations. The efficacy of preservatives depends on various factors, including substrate composition and interaction among the components of a specific formulation. Molecules such as phenoxyethanol (POE), caprylylglycol (CPG) and methylparaben (MEP) are widely used as preservatives in the food and cosmetic industries, however a molecular understanding of their interactions with surfactants and the kinetics of membrane partitioning remains unexplored. In this study coarse-grained molecular dynamics simulations were carried out to evaluate and quantify the kinetics of membrane partitioning for preservatives and surfactants in *Escherichia coli* membrane. We propose a mass transfer-based model to determine membrane partitioning kinetics of formulation constituents. Faster kinetics were observed for first order partitioning of POE and MEP ($\sim 0.01 \mu\text{s}$) when compared with zeroth order kinetics ($\sim 0.1 \mu\text{s}$) for CPG. In contrast surfactants such as sodium laureth sulphate (SLES) and cocamidopropyl betaine (CAPB) follow zeroth order membrane partitioning kinetics with significantly higher time constants. Interestingly, partitioning kinetics are influenced by the aggregation characteristics of constituents in bulk. Using a sequential micellar breakup model with single surfactant release kinetics we analytically recover this unique zeroth order membrane partitioning kinetics. When preservatives present in mixture, the kinetics of partitioning were found to decrease by a factor of 2-10. Significantly, the equilibrium membrane saturation coefficients for both preservatives and surfactant remained invariant in the mixtures due to the wide separation of timescales for surfactants and preservatives. The kinetic models developed in this study can be used to quantify membrane partitioning of preservatives and understand the influence of surfactants in specific formulations.

Understanding thermodynamic and kinetic properties of complex biomolecular systems employing molecular dynamics simulation

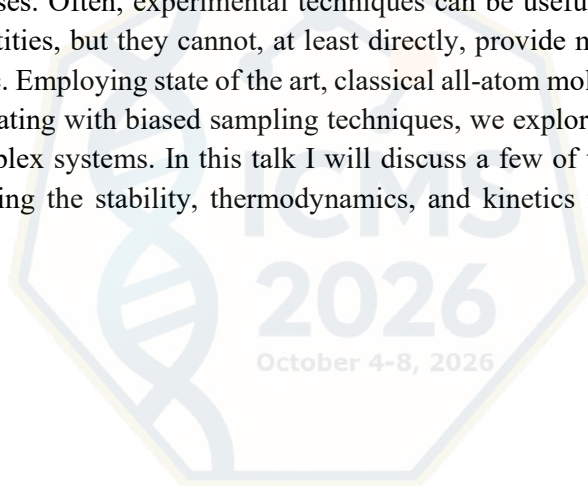
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Abstract

Understanding functionalities and mechanistic behavior of biomolecular systems such as protein – ligand and protein – DNA are highly desirable due to implication in basic biology as well as various diseases. Often, experimental techniques can be useful in measuring various thermodynamic quantities, but they cannot, at least directly, provide microscopic details and kinetics, pathways etc. Employing state of the art, classical all-atom molecular dynamics (MD) simulation and integrating with biased sampling techniques, we explore thermodynamics and kinetics of such complex systems. In this talk I will discuss a few of these methods and our efforts in understanding the stability, thermodynamics, and kinetics for different protein – ligand systems.



Class C Ice Nucleation and Growth Mechanism by Bacterial Ice Nucleating Protein

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Abstract

The bacterial ice-nucleating proteins (INPs) are the most efficient biological heterogeneous ice nucleators that can nucleate ice at -7.6°C or below, through class C nucleation, directly relevant for global climate due to their extreme environmental resilience and abundance [1]. Although monomeric INP can increase the water order through its ice nucleating sites, dimer is responsible for class C activity [2, 3]. Despite the years of extensive research, the molecular origin of a dimeric prerequisite for the class C ice nucleation and the precise mechanism remains elusive. Using all-atom molecular dynamics simulations of the INP, we show that tyrosine (Y) residues, present in hairpin-like conserved turns that connect opposite sides of the β -helix of the protein, serve as the primary ice nucleating site contrary to the previously predicted motifs [2, 4]. Hydroxyl groups of Y ladders from a side-wise anti-parallel dimer are bridged by interface water molecules that themselves template ice nucleus. Thus the dual functionality of dimerization and ice nucleation by Y in the hairpin domain drives the key mechanism of class C ice nucleation. On further cooling, the ice nuclei grow into fully formed stacking-disordered ice with coexistence of hexagonal and cubic ice. Together, our results explain why the dimer, not the monomer, is the minimal functional unit of class C bacterial ice nucleation along with the molecular pathways.

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First-principles molecular dynamics of excitons

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Abstract

To describe the excited state of an exciton within the framework of quantum molecular dynamics, this work uses the ROKS approach [1], which, due to its computational efficiency, offers unique opportunities for the direct study of the electron system with explicit consideration of finite-temperature lattice vibrations. Within the framework of this approach, exciton dissociation in dense hydrogen fluid [2] and polymerization in dense molecular nitrogen [3] have previously been described.

Developing the approach to describing excitons within the framework of quantum molecular dynamics to take into account finite-temperature lattice vibrations, in this paper the structure and transport of a light exciton in a MoS₂ monolayer were considered. Using the centers of the maximally localized Wannier functions, the correlated dynamics of the electron-hole pair forming the exciton was studied at different temperatures; the corresponding radial distribution functions with explicit Coulomb asymptotics were obtained, as well as the temperature dependence of the diffusion coefficient of the light exciton, from which the activation energy was determined [4]. In addition, in this report the radial distribution function for the dark exciton will also be considered.

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Understanding the Role of Entanglements and Crosslink Networks in Elastomer Performance

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Abstract

The mechanical performance of elastomeric materials is governed by a complex interplay between polymer chain architecture, entanglement networks, and chemical crosslinks formed during vulcanization. While crosslink density is widely recognized as a key parameter controlling stiffness and elasticity, the contribution of physical entanglements and their interaction with crosslink networks remain less understood, particularly in advanced tyre elastomers with varying chain flexibility and molecular structure. Developing a molecular-level understanding of these mechanisms is essential for designing rubber compounds with improved durability, strength, and energy efficiency.

In this work, molecular simulation approaches are employed to investigate the role of entanglements and crosslink topology in determining the structural and mechanical behavior of elastomer networks. Both atomistic and coarse-grained molecular dynamics models are utilized to examine the evolution of chain conformations, network connectivity, and deformation-induced structural changes across multiple length scales. Particular emphasis is placed on understanding how variations in polymer microstructure influence chain mobility, entanglement formation, network architecture, and stress transfer mechanisms under mechanical loading.

Our results reveal a counterintuitive inversion: chemical modifications that increase local chain flexibility can simultaneously enhance macroscopic tensile strength, which governs the effective network strand density and thereby the macroscopic elastic response. At the mesoscale, we employ coarse-grained MD to probe how crosslink density and chain stiffness jointly govern the equilibrium shear modulus across a range of network architectures. Specifically, we examine whether the classical additive decomposition of entanglement (G_e) and crosslink (G_x) contributions to the total modulus holds universally, or whether cooperative effects between physical and chemical network elements give rise to systematic deviations — characterized here as a function of crosslink density and chain rigidity.

These studies establish a coherent multi-scale picture of how chain architecture and network topology control elastomer mechanics, with implications for the rational design of high-performance rubber materials in tyre and industrial applications.

Density Corrected Many-body Methods and Kohn-Sham Functionals for Molecule Ionic Surface Interactions

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Abstract

Density-driven errors in Kohn-Sham (KS) density functional theory (DFT) represent a well-established source of inaccuracy in electronic structure calculations.^[1] A powerful remedy — replacing the self-consistent functional density with the Hartree-Fock (HF) density, yielding HF density-corrected DFT (HF-DC-DFT) — has demonstrated broad success for molecular systems.^[2] Here, we report the first application of HF-DC-DFT to molecule-surface interactions, using small-molecule adsorption on MgO(001). Employing the r²SCAN meta-GGA functional with D4 dispersion corrections evaluated on the HF density (r²SCAN-D4@HF), we achieve chemically accurate interaction energies across all systems tested, in excellent agreement with MP2+ Δ CC reference values. We further demonstrate that comparable accuracy can be obtained in a fully parameter-free framework through the perturbative-singles corrected random phase approximation (RPAS), here extended for the first time, from molecular dimers to periodic solid-state systems.^[3] Collectively, these results establish the critical role of density-driven error correction in describing molecule-surface interactions, and open a practical route to high-accuracy, low-cost modeling of surface adsorption phenomena.

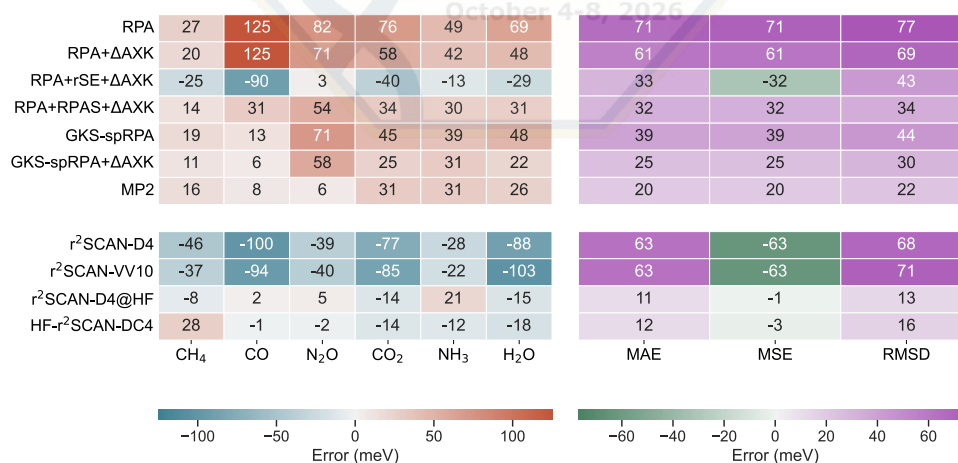


Figure 1: Errors in interaction energies for small-molecule–MgO(001) systems. MP2+ Δ CC method is used as the reference.

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Gold nanoparticle aggregation induced scrolling of boron nitride nanosheet

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Abstract

The nanoscale assembly of metallic gold nanoparticles on insulating boron nitride nanosheets gives rise to hybrid nanostructures, exhibiting novel synergistic properties that can be effectively harnessed for advanced sensing, catalysis, nanoelectronics, biomedical, and environmental applications. In the present study, the interfacial interactions between varying numbers (2, 4, 6, and 8) of gold nanoparticles and a single-layer boron nitride nanosheet have been systematically investigated using molecular dynamics simulations performed with NAMD package and suitable force-field parameters [1, 2]. Gold nanoparticles spontaneously aggregate and adsorb onto the boron nitride nanosheet, driven by attractive van der Waals interactions. At higher gold nanoparticle loadings (6 and 8 gold nanoparticles), the BN nanosheet spontaneously evolves into a scrolled configuration around the gold nanoparticle aggregate. The observed scrolling arises from the interplay between Au–BN interaction energy and the bending energy of the BN nanosheet, where the increased gold nanoparticle loading provides sufficient interaction energy to overcome the elastic resistance of the nanosheet.

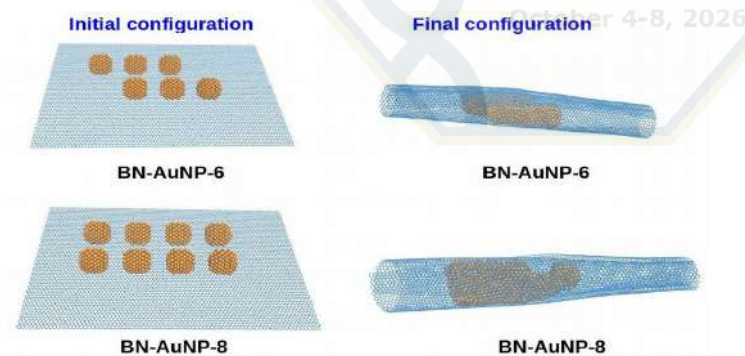


Figure 1: Initial and Final configuration of gold-boron nitride systems

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Selective Recovery of Uranyl Ions From Sea Water Using Covalent Organic Framework Membranes

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Abstract

Selective recovery of uranyl ions from aqueous environments is important for both uranium resource utilization and environmental remediation.¹ However, achieving high ionic selectivity in membrane-based separations without compromising water permeability remains a significant challenge. Herein, we employ molecular dynamics simulations to elucidate how covalent organic framework (COF) membranes can be engineered for selective uranyl transport. Slipped TpPa-1 and TpPa-F4 membranes exhibit complete rejection of UO_2^{2+} while allowing the passage of competing ions (Na^+ , Cl^- , and NO_3^-), whereas TpBpy and Tp-Azo exhibit only partial rejection. Both TpPa-1 and TpPa-F4 suppresses the transport of other divalent ions, such as Ca^{2+} and Mg^{2+} , pointing to a broader selectivity against multivalent species. Free energy calculations reveal that this selectivity originates from an energetic barrier of 3.6 kcal mol⁻¹ imposed by the bilayer pore environment, which selectively impedes multivalent ions without hindering the transport of water or monovalent ions. This mechanism remains effective in multilayer TpPa-1 membranes, demonstrating its robustness with increasing thickness. Collectively, these findings establish a clear structure-transport relationship in COF membranes and position slipped architectures as a viable route for uranium resource recovery and in mitigating uranium contamination in aquatic environments.

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AI assisted identification of low-energy conformers of mono- and di-saccharides and comparison with experimental vibrational spectra

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Abstract

Many experimental investigations have demonstrated the potential of using Infra-Red Pre-Dissociation (IRPD) spectra to resolve the structure of carbon-hydrates¹⁻³. The ability to efficiently explore the intricate 3D conformational space of carbohydrates with first-principles accuracy is crucial to extend the scope of above-mentioned success. To search the vast conformational space of mono- and di-saccharides, we integrate Deep-Learning Neural Network Potential (DL-NNP) with first-principles methods to develop "ab initio structure search" to boost the speed of structural search of complex sugars and peptides by more than one thousand times without losing first-principles accuracy⁴⁻⁶. Recently, we have benchmarked with available experimental IR(M)PD on mono- and di-saccharides and our preliminary results show that the computational scheme we demonstrate has sufficient accuracy⁶⁻⁸. We are optimistic that the integrated (experiment + simulations) approach can be used a promising tool for glycoscience.

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Machine-Learned Potentials for Simulating the Mechanics and Dynamics of Metal-Organic Frameworks

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Abstract

Understanding the structural responsiveness of metal-organic frameworks (MOFs), from breathing transitions and gas adsorption to high-temperature decomposition, demands simulations that are both chemically accurate and computationally efficient. Our recent work tackles this challenge by developing machine-learned interatomic potentials (MLIPs) that approach quantum-chemical fidelity at a fraction of the cost.

A natural starting point is gas adsorption, the very process that triggers many of the anomalous transitions observed in flexible MOFs. We have built MLIP-MC, an open-source framework that couples universal MLIPs with grand canonical Monte Carlo sampling, enabling adsorption simulations that go beyond the limitations of generic force fields.^[1] Benchmarking several universal models for CO₂ uptake in ZIF-8, ZIF-4 and Mg-MOF-74 reveals that prediction quality is governed not by model architecture alone but by the chemical diversity of the training data: only potentials exposed to MOF-adsorbate configurations during training reproduce DFT-level energetics. These insights provide a practical roadmap for reliable high-throughput screening of porous materials.

The same philosophy of learning potentials from first-principles data extends naturally to far-from-equilibrium processes. By fine-tuning foundational MLIPs on short ab initio trajectories and employing biased sampling to explore the relevant phase space, we have simulated the pyrolysis of CALF-20 and ZIF-8 over nanosecond time scales, orders of magnitude beyond the reach of direct DFT dynamics.^[2] The resulting trajectories capture linker decomposition, gas evolution and reorganisation of zinc coordination environments in full atomistic detail, offering a direct computational link between a precursor framework and the structure of its MOF-derived catalyst.

As the complexity and variety of these simulations grow, so does the need for intelligent orchestration. To this end we have developed QUASAR, an autonomous system in which a large language model plans, executes and analyses multi-scale atomistic workflows without human intervention.^[3] By unifying DFT, molecular dynamics and Monte Carlo under a single reasoning agent, QUASAR points toward a future in which the full cycle of computational materials discovery, from property prediction through to mechanistic understanding, can be carried out autonomously for coordination frameworks and beyond.

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Hybrid Sampling Machine-Learning Potentials for Accurate Hydrogen Adsorption in MOF-303

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Abstract

Metal-organic frameworks (MOFs) are promising candidates for hydrogen storage due to their high surface area and tunable porosity [1]. However, accurate computational prediction of gas adsorption isotherms and thermodynamics remains challenging. Classical force fields often lack accuracy, while *ab initio* molecular dynamics (AIMD) is computationally expensive for large-scale grand canonical Monte Carlo (GCMC) simulations. In this study, we propose a hybrid sampling workflow to develop robust machine-learning potentials (MLPs) capable of bridging this gap. We demonstrate this approach for hydrogen adsorption in MOF-303 [2].

We constructed a training dataset for MOF-303 by combining: (1) classical force-field (FF)-based GCMC snapshots evaluated with single-point density functional theory (DFT calculations) to cover high-energy insertion states, and (2) AIMD trajectories at multiple temperatures (77–900 K) to capture thermal equilibrium dynamics. The resulting dataset was used to train graph neural network potentials [3], which then were deployed to perform GCMC simulations for adsorption isotherms and molecular dynamics (MD) simulations for diffusion analysis.

The developed MLP achieves near-DFT accuracy and enables stable GCMC simulations. As shown in Fig. 1(a), our MLP-GCMC results at 298 K predict significantly higher H₂ uptake compared to those obtained with classical FFs and pretrained machine-learning potential (SevenNet-0 [3]) and are consistent with a calculated isosteric heat (~ 8.0

kJ/mol). Furthermore, by performing MLP-based MD simulation, the preferable adsorption sites are identified as shown in Fig. 1(b), where the iso-surfaces of H₂ probability indicate distinct primary and secondary adsorption sites, localized near the polar N/O motifs, confirming the role of specific chemical environments in stabilizing hydrogen.

We established a hybrid sampling framework that generates robust MLPs for gas adsorption. The resulting potential accurately reproduces thermodynamic properties and reveals microscopic adsorption and diffusion mechanisms in MOF-303. This workflow provides a generalizable tool for the high-throughput screening of porous materials for energy applications.

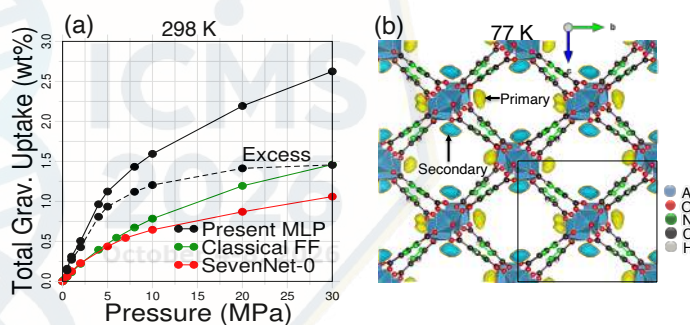


Fig. 1 (a) Calculated H₂ adsorption isotherms for MOF-303 using different potential models. (b) Three-dimensional iso-surface plots of H₂ probability density, highlighting the spatial distribution of primary and secondary adsorption sites within the pore.

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Correlating structures, dynamics and thermodynamics of molecular system in bulk, at interface and under confinement

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Abstract

A fundamental understanding of structures, dynamics and thermodynamics of molecular system in bulk, at interface and under confinement is of immense important in the various fields of science and technology. The experimental techniques for obtaining these characteristics are rather challenging and sometimes not obtainable. Ab-initio and classical molecular dynamics simulations have been and are being used to compliments the experimental findings and some cases are used to predict the molecular characteristics which are beyond experimental reach. The present talk will deliberate the structures (radial distribution function), dynamics (diffusion and viscosity) and thermodynamics (entropy) of molecular system in bulk, at interface and under confinement and their unique correlations.

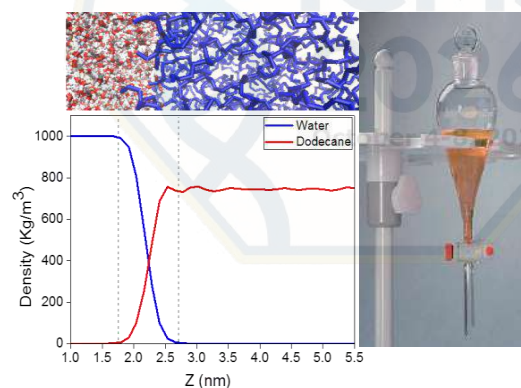


Figure: Computer simulated interface of water-dodecane bi-phasic system.

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Chemically Intuitive Equivariant Graph Neural Networks for Directional Property Learning

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Abstract

Deep learning models based on graph neural networks (GNNs) have demonstrated strong performance in predicting molecular properties. However, most approaches primarily focus on scalar quantities and rely on rotation-invariant representations. This limits their ability to capture inherently directional physicochemical properties. Recent advances in three-dimensional GNNs such as SchNet incorporate geometric information but remain largely restricted to invariant predictions.^[1] In contrast, equivariant frameworks including PaiNN explicitly preserve rotational symmetry and have shown improved physical consistency in modeling molecular systems.^[2]

In this work, we present an equivariant graph neural network framework that enables the direct learning of vectorial properties in three-dimensional molecular systems. By jointly propagating scalar and vector features through message passing, the model captures the intrinsic relationship between molecular structure and directional properties such as dipole moments. Notably, despite being trained only on scalar targets, the model successfully recovers consistent directional information. This result suggests that embedding fundamental chemical principles into the model architecture leads to physically meaningful representations.

Benchmark evaluations demonstrate that the proposed approach outperforms conventional rotation-invariant and rotation-variant GNN models in dipole moment prediction tasks. The model also maintains strong performance on standard scalar property datasets. In addition, analysis confirms that the model preserves rotational equivariance and accurately reflects changes in molecular orientation without loss of consistency. This behavior is essential for reliable modeling of three-dimensional chemical systems.

Beyond molecular systems, this framework provides a promising pathway toward extending equivariant learning to materials and surface science. As a preliminary step, ongoing work explores the application of the model to simple slab-based systems. The goal is to investigate surface-dependent properties and reconstruction phenomena under realistic conditions. This direction highlights the potential of physically grounded machine learning approaches in bridging molecular-level understanding and complex material interfaces.

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AI and Foundation Model–Driven Prediction of Critical Micelle Concentration in Surfactant Systems

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Abstract

Accurate prediction of critical micelle concentration (CMC) is essential for understanding surfactant behaviour across diverse chemistries and compositions. However, conventional modelling approaches are often limited in their ability to generalize across different surfactant classes and mixture combinations, particularly in data-constrained settings.

In this work, we present a data-driven modelling framework for predicting CMC across pure surfactants and binary surfactant mixtures. The approach leverages a combination of molecular descriptors, learned embeddings, and neural network architectures to capture structure–property relationships governing micelle formation. Multiple modelling strategies were explored, including descriptor-based models and embedding-driven neural networks, to evaluate performance and generalization across chemical space.

The developed models demonstrate strong predictive performance for pure surfactants ($R^2 \sim 0.89$), with extension to binary mixtures achieved through combined surfactant representations that enable generalization across compositions. Model interpretability is incorporated using SHAP analysis, linking predictions to key molecular features such as hydrophobicity, polar surface area, and molecular flexibility.

Foundation model–derived representations are further explored to enhance molecular encoding beyond traditional descriptors, enabling improved generalization in low-data regimes and across diverse surfactant chemistries.

Overall, this work highlights the potential of deep learning and foundation model approaches to build robust, generalizable models for predicting CMC in surfactant systems.

Reconciling Theory and Experiment

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Abstract

Despite advances in (bio)physical techniques it is still not possible to directly observe the energetic and dynamic properties of individual atoms in (bio)molecular systems using experimental approaches. Everything we think we know regarding (bio)molecular systems at an atomic level is to some extent a model. The question is to what extent can the models used to interpret experimental data be trusted and to what extent uncertainties in experimental data bias the models we use to understand how molecules interact. For example, while the overall structure of a protein may be resolved in near atomic detail, the position, orientation and/or conformation of a small molecular ligands (cofactors, inhibitors etc.) are often much less certain. Historically, electrostatics have been ignored in structure refinement, yet these potentially flawed structural models are now central to determining if new predictions are correct. There is also systematic bias in how experimental data is used or interpreted. The variation in area per lipid in theoretical calculations of membrane systems is much less than that measured experimentally. This is not only a problem for experimentalists but represents a fundamental challenge to theoreticians attempting to develop and validate new computational models. Using a range of examples, I will illustrate how different theoretical or structural models bias our interpretation of data, but how, when used appropriately, molecular simulations with well validated force fields, provide a unique means to challenge our interpretation of experimental data leading to increased certainty in some cases, new insights into the true nature of (bio)molecular systems in others.

The Birth, Life and Death of an Ion: Faradaic Charge Dynamics in a Nanoconfined Electrochemical Cell

Tod A Pascal

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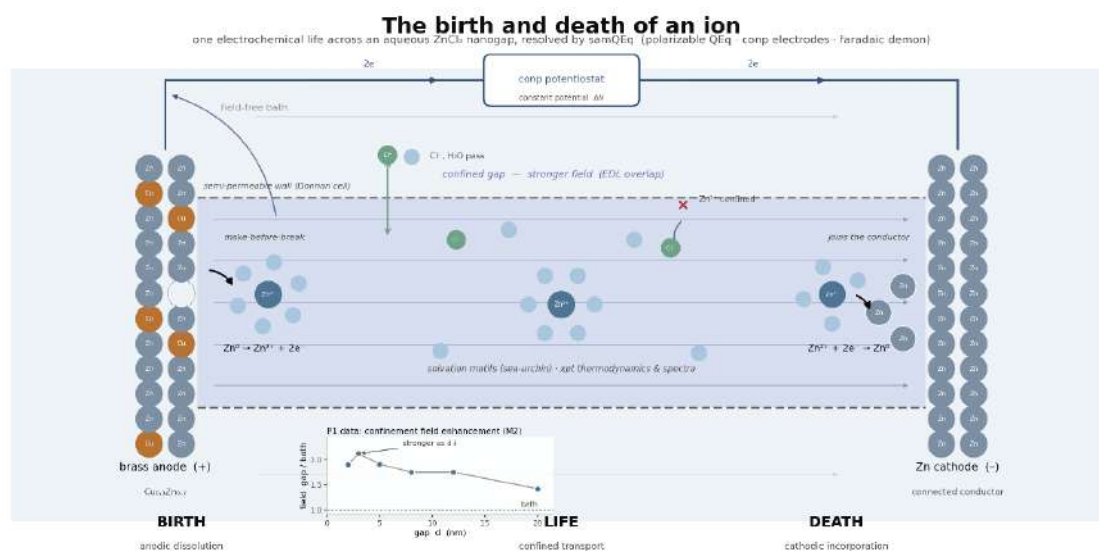
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Abstract

An ion in an electrochemical cell has a rich and sometimes complex life. It is born when a metal atom gives up its electrons and steps off the lattice into solution; it lives as a solvated, transported, screened charge; it dies when it accepts electrons back and rejoins a metal electrode. Simulations have long treated these as separate problems handled by separate methods. We present a single framework, samQEq, that carries the ion through all three. We incorporate polarizable charge-equilibration molecular dynamics — where atomic electronegativity and hardness play the role of frontier-orbital levels — with constant-potential electrodes (a computational potentiostat) and an explicit faradaic Monte-Carlo kernel that proposes integer electron transfers between electrode and ion, accepting them by Metropolis on the full-system energy difference. The proposal kernel is reversible and satisfies detailed balance: a demon in spirit, but thermodynamically honest. This unification exposes electron-transfer-mediated physics inaccessible to separate treatments.

Each act in the ion's lifespan carries its own physics. At birth, oxidation is a compound oxidize-and-displace move that lifts the atom off the lattice into its first hydration shell; the underlying kinetics reproduce two-state Nernstian equilibrium quantitatively (slope 38.72/V against the theoretical 38.68). Applied to $\text{Cu}_{0.3}\text{Zn}_{0.7}$ dealloying in a full two-electrode loop, the same kinetics yield a bimodal distribution of parting-limit behavior. During its life in the electrolyte, we classify the first solvation shell using unsupervised learning, and show that each solvation structure has a distinct Raman signature, with thermodynamic stabilities that vary down the aquo-to-chloro ladder as chloride concentration rises. Near death, reduction retypes the ion into the metal and it joins the growing conductor's connected component, floating at the electrode potential. This event is shown to have an unambiguous electronic signature, revealed by simulated total electron yield X-ray adsorption spectroscopy.

Nanoscale confinement reveals even more interesting physics. A species-selective wall holds Zn^{2+} between two immersed electrodes while water and Cl^- exchange freely with the bath — a Donnan cell. The 2–20 nm gaps sustain a $1.4\text{--}2.1\times$ stronger field than the bath, strengthening as the gap narrows. We present the confinement-resolved equilibrium potential, Tafel kinetics and intrinsic Marcus barriers, the crossover between bond-breaking and EDL-migration control, and gap-bridging morphology, organized by a single control parameter, d/κ^{-1} — the gap measured in Debye lengths. The result is electrochemistry resolved at the scale where batteries, separators, and biological channels actually operate: one ion at a time.



Molecular Superfluidity in Doped Parahydrogen Clusters

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Abstract

A hydrogen molecule consists of two protons and two electrons. In the adiabatic approximation, the wave function is separated into components corresponding to electrons, vibration, rotation, and nuclear spin. Hydrogen molecules with even rotational quantum numbers are termed parahydrogen, while those with odd numbers are orthohydrogen. Transitions between these states are rare on laboratory timescales, so they are treated as distinct chemical species. At low temperatures, only parahydrogen with a quantum number of 0 is typically observed. Because a hydrogen molecule is made of an even number of fermions, it follows Bose-Einstein statistics. Due to its low mass, the molecule's wave properties are evident at low temperatures, potentially leading to a superfluid phase, as in helium-4. The hydrogen triple point is at 13.8 K, and no superfluidity is observed down to this temperature. Ginzburg et al. proposed in the 1970s that superfluidity might occur in a supercooled state, estimating a transition temperature around 6 K via a simple argument [1]. Even when the temperature is lowered carefully, liquid hydrogen in its supercooled state crystallizes before reaching superfluid conditions. Small clusters might sustain a "liquid state" at very low temperatures, and the superfluidity of helium clusters has been extensively studied [2]. Using our path-integral hybrid Monte Carlo method [3-5], we investigated the structure and superfluidity of methane-doped parahydrogen clusters at low temperatures. For experimental results associated with this system, see reference [6].

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TITLE: Developing Simulation Techniques to Study Crystal Nucleation of Solutes from Solutions

ABSTRACT

While techniques for simulating crystal nucleation from melt are mature and well established, the same cannot be said for simulating crystal nucleation from solutions. There is a fundamental difference between the chemical physics for nucleation from a solution compared to that from a melt. In a melt, the dominant process for crystal nucleation is the rearrangement of molecules to form. In contrast, the dominant process for nucleation from a solution is the slow diffusion of solute molecules from the bulk to the interface of the nucleus. The other main technical challenges include (i) computational expense to simulate large number of solvent molecules and (ii) necessity to maintain solute concentration in the bulk during formation of a crystal nucleus. In this talk, I will present the ongoing efforts in our group towards addressing the above challenges. These include (i) development of a molecular theory of nucleation for solute crystallization, (ii) identification of important collective variables to efficiently bias the formation of a nucleus, and (iii) use of finite temperature string method to compute the nucleation pathway. I will use examples from aqueous solutions of NaCl, CaCO₃, and methane (for gas hydrates) to illustrate the above points.



Optical properties, Electron-phonon coupling and Spin fluctuations in 2D Quantum Materials

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Abstract

Two-dimensional quantum materials such as MoSe₂, and other transition metal dichalcogenides (TMDs) are reputed for atomically thin spintronic, valleytronic and topological devices. With the advent of exascale computing, an exploration into the topological manifestation in 2D materials have been deemed indispensable. Functional two-dimensional materials are promising for advanced atomically thin electronic and optoelectronic devices, such as light emitting diodes (LEDs), ultrathin solar cells, and valleytronic devices. Recently, atomic layers of oxides^[2] and hexagonal Si/Ge have been successfully grown using micromechanical and sonochemical exfoliation. We performed first-principles calculations based on density functional theory and many-body perturbation theory to investigate the electronic and optical properties (utilizing the GW and BSE methodology) of monolayer, bilayer, and bulk litharge. Further, we have investigated the phonon lifetimes and linewidths, Gruneisen parameters and Raman modes in layered hexagonal phases of Si/Ge. A latest addition to the landscape of exotic 2D materials pertains to the discovery of not yet foretold superconducting state in monolayers of NbSe₂ dubbed ‘Ising superconductivity’. In our study, we have investigated the energetics, magnetic moment and fully q-dependent spin susceptibility in order to pin point the location of the ferromagnetic instability in the Brillouin zone of this material. This involves our methodology of inverting the random-phase approximation, and utilization of first principles calculations artificially stabilized by Hubbard interactions and spin-spiral calculations for evaluation of the fluctuation renormalized spin susceptibility. The role of spin fluctuations and electron phonon coupling in determining the superconducting order parameter for the newly popular 2D Ising superconductor NbSe₂ will be discussed.^[1]

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Quantum Embedding for Correlated and Excited-State Phenomena

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Abstract

Accurate electronic-structure simulations of complex molecular and materials systems are often limited by the steep computational scaling of correlated wavefunction and many-body methods. In many applications, however, the electronic phenomenon of interest such as strong correlation, an optical excitation, or a nonlinear response, is localized within a comparatively small region, while the surrounding environment primarily modifies its electronic structure. Quantum embedding exploits this locality by treating the chemically relevant subsystem with an accurate high-level method and the remaining environment at a computationally efficient density functional theory (DFT) level.

We present the development and implementation of density-based quantum-embedding methods for molecular and periodic systems in the TURBOMOLE program package^[1-3]. The total system is partitioned into active and environmental subsystems coupled through an embedding potential, enabling advanced electronic-structure methods to be applied selectively to the active region. The framework has been interfaced with correlated wavefunction theory, many-body perturbation theory, and real-time time-dependent DFT (RT-TDDFT), providing access to both ground- and excited-state properties of complex systems at substantially reduced computational cost.

Applications include the calculation of absorption spectra of molecules in explicit solvent environments, where correlated wavefunction-in-DFT embedding reproduces the environmental shift in molecular excitation energies without requiring a correlated treatment of the complete solvent system. RT-TDDFT coupled with embedding further enables the simulation of nonlinear light-matter interactions, including the influence of condensed-phase environments on molecular high-harmonic generation. For periodic materials, cluster-in-periodic embedding makes it possible to describe localized excitations, adsorption phenomena, and correlated electronic states using high-level methods while retaining the extended crystalline environment.

In the recent years, quantum computing algorithms like the variational quantum eigensolver (VQE) have emerged as a promising route for treating strongly correlated electronic systems on the current quantum hardware. However, VQE is still not feasible for larger molecules or periodic systems. To circumvent these limitations we have extended the embedding framework and developed a VQE-in-DFT approach in TURBOMOLE. This classical-quantum embedding strategy provides a pathway for applying near-term and future quantum-computing methods to realistic chemical and materials environments without representing the complete system on a quantum device.

Complementing these embedding developments, we have created PyFock^[4], an open-source Gaussian-basis Kohn-Sham DFT code written in Python and accelerated for multicore CPUs and GPUs through just-in-time compilation and GPU-enabled numerical kernels. To the best of our knowledge, PyFock is the first Indian-developed Gaussian-basis DFT code with GPU acceleration. Its transparent architecture, density-fitting implementation, exchange-correlation integration, and CPU/GPU back ends make it suitable for both electronic-structure calculations and rapid methodological prototyping.

Together, these developments establish a multilevel computational strategy in which classical DFT, correlated electronic-structure methods, GPU acceleration, and quantum algorithms are combined to address correlated and excited-state phenomena in complex molecular and materials systems.

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Multi-scale molecular dynamics simulations of biomolecular condensates

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Abstract

It has been suggested that droplets formed within cells through liquid-liquid phase separation serve as platforms for many biological phenomena, such as signal transduction, but also act as precursors to aggregates believed to underlie conditions such as neurodegenerative diseases. For this reason, the formation and dissolution of vesicles are key targets in computational chemistry. The interiors of droplets contain many flexible molecules, such as natively denatured proteins and RNA, which maintain a highly concentrated, fluid state through multivalent interactions. We have conducted computational research to elucidate the conditions necessary for droplet dissolution using multiscale molecular dynamics (MD) simulations. Since droplet formation and dissolution are slow biological processes, it is difficult to capture the essential processes using all-atom MD alone. Therefore, it is efficient to perform MD calculations using a coarse-grained (CG) molecular model that approximates amino acid residues as a single particle. However, factors not included in CGMD—such as the details of the solvent, ions, and intermolecular interactions, as well as the role of transient secondary structures—are important for understanding the molecular mechanisms of droplet formation and dissolution. Therefore, by converting (back-mapping) the molecular structures obtained from CGMD to all-atom models and then performing all-atom MD, it is possible to simultaneously achieve efficient conformational sampling and detailed analysis of intermolecular interactions. We applied this multi-scale approach to analyzing droplet formation and dissolution involving several intrinsically disordered proteins.

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Understanding the Action of Pore Forming Proteins: Insights from Molecular Dynamics and Free Energy Computations

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Abstract

The plasma membrane of our cells form the first line of defence to external threats. Protein-membrane interactions dominate this landscape, playing an important role in our understanding of a myriad of bacterial and viral infections. Pore-forming toxins a subclass of proteins expressed by bacteria form their primary arsenal responsible for over 30 % of bacterial infections. Pore forming proteins/toxins expressed in a water-soluble form bind to the target cellular membrane and self-assemble to form multimeric transmembrane pore complexes to eventually kill the cell. In this talk I will summarize our understanding of the pore forming toxin cytolysin A (ClyA) – a 34 kDa protein expressed by *E. coli* and known to undergo one of the largest conformational transitions during pore formation. We use large scale molecular dynamics simulations at atomistic and coarse grained levels and enhanced free energy sampling methods in combination with experiments on supported bilayer and vesicle platforms to unravel the process of membrane insertion and kinetics of pore formation. Each of the different techniques offers unique insights at different length and time scales into membrane binding, influence of lipid composition as well as the inherent conformational changes that the protein undergoes during the pore formation process. We connect membrane insertion and ensuing conformational changes with recent superresolution and single molecule microscopy data to provide molecular insights into the pore forming pathway.

Elucidating the role of hierarchical dynamics in biomolecules: From chemical reactions to functions

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Abstract

Structural fluctuations and conformational transitions are ubiquitous features of proteins and are essential for their functions. Experimental techniques such as single-molecule FRET and NMR relaxation dispersion measurements have provided valuable insights into these dynamic processes. However, a comprehensive understanding of how conformational dynamics contribute to protein function remains elusive. While molecular dynamics (MD) simulations offer atomistic details of equilibrium conformations and transition pathways, traditional studies have mostly focused on static thermodynamic quantities such as free energy landscapes and kinetic rates while omitting the dynamic aspect.

In this talk, I will discuss how the hierarchical dynamics of proteins occur and contribute to the function of proteins. In the enzyme catalysis, the conformational transitions in the protein precede the chemical reaction. This temporal separation between protein and ligand dynamics is attributed to their differing spatial and temporal scales. Notably, the reactive protein conformation, i.e., conformational excited state, emerges as a transiently populated state prior to the chemical reaction events.^[1] Furthermore, by analyzing the slow dynamics of the enzyme, the equilibrium distribution of conformational ensembles is found to shift after the chemical reaction. This redistribution creates an apparent coupling between protein dynamics and the chemical step that can be observed in NMR measurements, even though they occur on distinct timescales. In the circadian clock protein KaiC, the rate of ATP hydrolysis and phosphorylation/dephosphorylation states are found to oscillate in a circadian (~24 hour) period. By studying the mechanism of phosphorylation step, I will discuss how protein-protein interaction regulates chemical reactions and how chemical reactions reshape protein dynamics to regulate circadian rhythms in protein complexes.^[1]

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Proton-Coupled Hydride Transfer and Proton Relay Mechanisms in the Oxidation of Cholesterol by Cholesterol Oxidase (ChOx)

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Abstract

Cholesterol oxidases (ChOxs) are bifunctional flavoenzymes that catalyze the conversion of membrane-associated cholesterol into cholest-4-en-3-one (also simply referred as cholestenone) through two sequential half-reactions, namely the oxidation of the 3 β -hydroxyl group to yield cholest-5-en-3-one, followed by isomerization to cholestenone.^[1] These monomeric enzymes, which are unique to bacteria, are secreted by a variety of microbes that exclusively use cholesterol as their carbon and energy source. The oxidation of cholesterol to cholest-5-en-3-one involves two chemical events, a proton abstraction from the 3 β -hydroxyl group of the substrate and a hydride transfer from the substrate C3 position to the flavin N5 position.

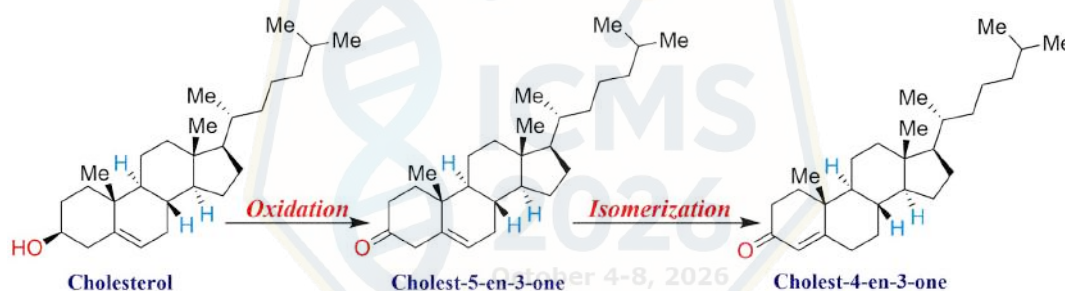


Figure 1: The oxidation of cholesterol to cholestenone occurs in two sequential steps, first being the oxidation of cholesterol to cholest-5-en-3-one and the second being the isomerization of cholest-5-en-3-one to cholest-4-en-3-one.

In here, we report a systematic Density Functional Theory (DFT) and Ab Initio Molecular Dynamics (AIMD) investigation coupled with Metadynamics (MTD) on deciphering the role of base and base strength in modulating the energy barriers and mechanistic pathways using truncated model systems.^[2]

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Title: Origin of internal friction in ring-flip in Cytochrome C

Authors: Bikirna Roy and Arnab Mukherjee

Abstract: Aromatic amino acids buried inside folded proteins play a critical role in stabilizing both the folded conformation and anchoring any incoming substrate molecules. Moreover, their ring flips serve as sensitive probes of protein breathing motions. In this work, we accurately estimate the ring-flipping rates of a phenylalanine residue in cytochrome C using metadynamics combined with reactive flux and Grote-Hynes theory. We show that the delayed response of cavity residues that provide steric hindrance to ring rotation manifests as memory-dependent friction. Increasing solvent viscosity slows the fluctuations of these cavity residues, reinforcing the delayed response and producing a fractional viscosity dependence of the flip rate, despite the ring being completely buried.



Decoding the Molecular Grammar of Heterotypic Biomolecular Condensates: Interplay of Sequence Architecture and RNA-Mediated Competitive Interactions

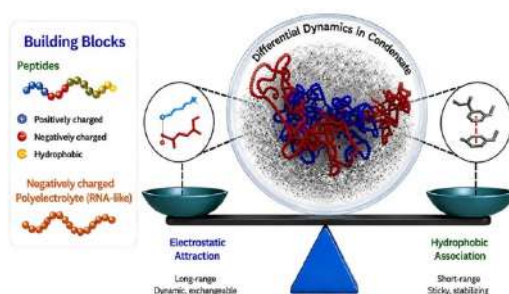
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Abstract

Biomolecular condensates formed through liquid–liquid phase separation organize cellular biochemistry by dynamically compartmentalizing proteins and nucleic acids without membrane boundaries^{1,2}. A central challenge is to understand how molecular sequence and RNA collectively encode the stability, dynamics, and material properties of these multicomponent assemblies. In this talk, I will present a unified computational framework that uncovers the molecular grammar governing heterotypic biomolecular condensates. Using coarse-grained molecular dynamics simulations, we demonstrate that sequence charge patterning acts as an intrinsic design principle, dictating condensate stability, intermolecular organization, and molecular transport³. Extending this framework, we reveal that RNA-like polyelectrolytes exhibit a remarkable dual role governed by the underlying interaction landscape. While RNA destabilizes electrostatically driven condensates through enhanced long-range repulsion, it stabilizes hydrophobic condensates by acting as a multivalent interaction scaffold that strengthens intermolecular connectivity. This competition between long-range electrostatic and short-range hydrophobic interactions gives rise to tuneable condensate morphology, dynamics, and emergent material properties. Together, these findings establish a predictive molecular framework linking sequence architecture and RNA-mediated regulation, providing fundamental insight into the physicochemical principles underlying cellular condensates and offering design rules for engineering programmable biomolecular materials⁴.



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From Autophagy to Mitochondrial Protein Sorting: Molecular Simulations Reveal Dynamic Mechanisms Governing Membrane-Associated Protein Complexes

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Abstract

Peripheral and integral membrane protein complexes must rapidly assemble and interpret molecular signals to coordinate essential cellular processes, including autophagy and mitochondrial protein sorting. These events are frequently orchestrated by highly flexible loops, intrinsically disordered regions (IDRs), and transient structural elements, making their molecular mechanisms exceptionally difficult to resolve using conventional structural biology approaches. Here, we present two complementary case studies in which multi-microsecond atomistic molecular dynamics (MD) simulations and Hierarchical Chain Growth (HCG) modeling bridge biochemical observations with nanoscale mechanistic insights, revealing how conformational dynamics regulate membrane-associated protein function.

In the first study^[1], we elucidate how the human autophagy-initiating ULK1 complex (ULK1C) targets membranes downstream of production despite lacking conventional lipid-binding domains. MD simulations of a complex assembly—comprising the HORMA dimer (ATG13 and ATG101) of ULK1C and PI(3)P-binding WIPI proteins—revealed a coplanar stabilization mechanism where the complex aligns flat to insert a protruding (Trp-Phe) WF finger of ATG101 directly into the bilayer. Furthermore, HCG modeling revealed that docking of a short (Pro-Val-Pro; PVP) motif within the extensive IDR of ULK1 onto ATG13 brings the catalytic kinase domain closer to the membrane, reducing its spatial exploration volume eight-fold and thereby accelerating substrate phosphorylation.

In the second study^[2], we investigate how the mitochondrial inner membrane translocase (TIM23 complex) deciphered topogenic signals to sort incoming precursor proteins for lateral bilayer insertion versus matrix transport. Using an *in vivo* fluorescence sensor (FLASH), we identified that the oxidoreductase introduces a critical intramolecular disulfide bond (Cys10-Cys77) into TIM17 of the TIM23 complex. Atomistic MD simulations under a physiological membrane potential revealed that this disulfide acts as a structural clamp, rigidly positioning an charge cluster to form an electrostatic permeability filter that arrests translocation via repulsion of stop-transfer signals. Quantitative depth distribution analysis confirmed that disrupting this clamp or the aspartate filters causes the substrate to slide vertically downward by into the matrix, completely bypassing lateral translocation.

Together, these studies highlight the broad impact of molecular simulations in identifying how IDR docking, atomistic filters, and structural clamps establish precise nanoscale mechanical switches governing macromolecular targeting and selectivity at complex biological membranes.

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Interpretable AI for Organic Reaction Prediction

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Abstract

The Reliable prediction of chemical reactivity still largely depends on the expertise of synthetic chemists. Automating this process with artificial intelligence could greatly accelerate synthesis design in future digital laboratories. Although recent machine learning models have shown promising performance, many rely on language-based representations that are difficult to interpret and differ from how chemists reason about reactions through electronic changes. Reaction mechanisms, which describe electron movements, are especially important for understanding kinetics and identifying unexpected products. In this talk, I will present our recent efforts to learn organic reactivity using chemical rules and algorithms^[1-7], with a focus on Reactron, an electron-based machine learning model for general reaction prediction. Reactron explicitly incorporates electron movements and generates arrow-pushing diagrams that describe the mechanistic steps leading to product formation. I will discuss its predictive performance compared with existing product-only models, its ability to adapt to new reactivity from only a few examples, and its use in exploring combinatorial reaction spaces for reaction discovery.

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Foundation models for materials simulation and design: where are we now?

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In recent years, AI approaches have attracted increasing attention in materials simulation. In particular, foundation models trained on large and diverse datasets are emerging as powerful tools for materials design. In this talk, I will review the current performance of foundation models for materials simulation and discuss strategies to improve their accuracy and applicability.

First, I will show that recently developed universal machine-learning interatomic potentials (uMLIPs) can already describe the potential energy surfaces (PESs) of nanomaterials in realistic environments with good accuracy, even in out-of-distribution chemical spaces. I will then discuss how their accuracy can be further improved using forgetting-aware fine-tuning methods. In addition, I will present approaches to accelerate materials simulations based on uMLIPs.

In contrast, our benchmark tests on diffusion models for materials design show a different trend. While these models perform well in well-sampled chemical spaces, their performance significantly deteriorates in under-sampled regions, such as systems containing rare-earth elements or structures with large unit cells. This discrepancy is intriguing because MLIPs and diffusion models are often trained on similar datasets and share related neural network architectures. To explain this behavior, I will introduce the concept of the “curse of periodicity,” which provides a theoretical perspective on why extrapolation in periodic crystal generation can be fundamentally challenging.

Hydration Environment of Complexes and Their Dynamics in Aqueous Zinc Chloride Solutions

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Aqueous ZnCl_2 serves as a model electrolyte where the zinc ion exhibits variable coordination geometries and strongly polarizes water in its solvation shells. Molecular dynamics simulations using a machine-learned interatomic potential trained at the revPBE-D3 level of density functional theory reveal its structure, dynamics, and electrostatics. Dilute solutions feature the dominant octahedral $[\text{Zn}(\text{H}_2\text{O})_6]^{2+}$ complex, which adapts to trigonal bipyramidal and tetrahedral geometries to accommodate chloride ions. Relative to bulk water, water molecules in zinc's first solvation shell in the complexes exhibit an enhancement of their dipole moment by 15–30%, and a retardation of their residence and reorientational time scales. The residence time displays a nonmonotonic dependence on the number of participating chloride ions; a minimum of 96 ps for $[\text{ZnCl}]^+$ and maxima of 550 ps for Zn^{2+} and $[\text{ZnCl}_3]^-$ are observed. Exchange and reorientation time scales in the second solvation shell decrease monotonically with chloride inclusion in the complex.



Learning Quantum Dynamics: AI-Driven Discovery of Structure–Property Relationships in Excited-State Materials

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Abstract

The discovery of next-generation optoelectronic materials increasingly depends on our ability to understand and predict excited-state processes across multiple length and time scales. However, direct first-principles simulations of ultrafast quantum dynamics remain computationally prohibitive, limiting our ability to explore complex materials and uncover design principles. In this talk, I will demonstrate how physics-informed AI can bridge this gap by learning atomistic structure–property relationships directly from ab initio simulations. First, I will present Atomistic Line Graph Neural Network (ALIGNN) models that predict femtosecond-resolved electronic properties of metal-rich CdSe semiconductor quantum dots with meV-level accuracy using only a small fraction of the available training data.^[1] Coupled with ensemble and transfer learning, these models enable long-time-scale predictions of band-edge dynamics and reveal how ligand chemistry governs vibronic coupling and transient trap-state formation. A Feature Nullification Analysis framework further provides atom-resolved interpretations, connecting specific atomic environments to transient electronic properties. Next, I will show how machine learning models, including artificial neural networks and information-theoretic analyses, accelerate the study of hot-carrier dynamics in Cs₂AgInX₆ (X = Br, Cl) halide double perovskites.^[2] Trained on only ~10% of first-principles data, these models accurately interpolate dynamic electronic properties and nonadiabatic couplings over extended trajectories, enabling reliable identification of subtle correlations between structural fluctuations and carrier relaxation pathways. The resulting insights explain the intrinsically prolonged hot-electron lifetimes in these materials and establish design principles for hot-carrier optoelectronics. Together, these studies illustrate a broader paradigm in which interpretable and data-efficient AI models serve not merely as surrogates for expensive simulations, but as scientific tools for uncovering hidden mechanisms in excited-state materials and accelerating the inverse design of next-generation optoelectronic systems.

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Data-Driven Approach to Derive Polymorph-Specific Order Parameters for Crystal Nucleation

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Abstract

The formation of stable crystals from a metastable solution, known as crystal nucleation, which plays a vital role in the pharmaceutical, chemical, and food processing industries. The outcome of the nucleation process is influenced by factors such as temperature, solute concentration, additives, and solvent. Different molecular arrangements lead to the formation of crystal polymorphs with distinct properties. Producing the correct polymorph is essential for use in the pharmaceutical industry. Since nucleation is an activated process, overcoming free-energy barriers in brute-force molecular dynamics (MD) simulations is infeasible except at very high supersaturations. Several methods were developed to address the time-scale issue, such as enhanced and path-sampling methods. However, these methods heavily rely on the choice of order parameters (OPs). Classical OPs, such as Steinhardt's, work well for atomic systems and simple molecules.[1] However, they fail to distinguish the crystal polymorphs comprised of flexible molecules.[2] Modified bond-orientational OPs and quaternions have been used for systems like glycine[3] and urea [4], but they remain system-specific. In this regard, we propose to use a machine learning approach to develop OPs that can not only distinguish the crystal from the solution phase but also distinguish among competing polymorphs. Initially, we worked with simple systems such as LJ and water to validate our approach. Then we extended our approach to complex molecules like orcinol, which exhibit the full range of polymorphic behavior one can expect in molecular crystals, making it ideal for such an investigation. We have considered two anhydrous forms of orcinol crystals along with the melt for our analysis. In this regard, we worked with both supervised and unsupervised learning to derive OPs for crystal polymorphs. This data-driven approach to predict accurate OPs will certainly help the crystal nucleation community to gain better insights into the nucleation process.

October 4-8, 2026

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What Do Deep Neural Networks Find in Disordered Structures of Glasses?

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Abstract

Glass transitions are widely observed across diverse soft matter systems. Yet despite decades of extensive research, the physical mechanisms underlying these transitions remain elusive. A central open question is whether the glass transition is associated with a diverging correlation length of characteristic static structures ^[1,2].

In this study, we develop a deep learning-based method to extract characteristic local structures directly from instantaneous particle configurations, without recourse to any dynamical information. We train a convolutional neural network (CNN) to classify configurations as either liquid or glass, and then apply gradient-weighted class activation mapping (Grad-CAM) to identify the structural features driving this classification by highlighting the regions most influential in the network's decision-making. Applying this framework to two model glass-forming liquids and comparing the results against several established structural indicators [2], we confirm that our method successfully captures system-specific structural features. We further find that the extracted structures exhibit strong correlations with long-time particle displacements ^[3,4].

From a methodological standpoint, earlier CNN-based approaches ^[3,4] and conventional structural indicators ^[2] alike required manual coarse-graining of the structural indices obtained. Our updated method addresses this limitation by employing a graph neural network (GNN), which improves computational efficiency and simultaneously enables automatic coarse-graining of structural information ^[5]. Our results suggest that structural features—hidden within disordered configurations yet revealed through these approaches—play a significant role in the glass transition.

Finally, we shall also discuss the application of this research to cancer cell lines. In particular, we shall demonstrate that it can be applied to the problem of isolating highly metastatic cells based solely on their cellular structure.

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Multiscale modeling of water transport and hydrolytic degradation of polymers

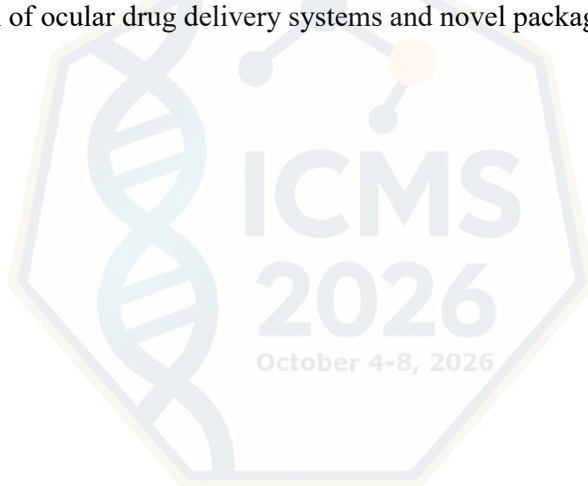
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Abstract

Research in biodegradable polymers has taken pace in last few decades due to their use in drug delivery systems and as sustainable alternatives to conventional plastics. Intelligent design of these systems requires an understanding of water transport through polymers and associated hydrolytic degradation processes. I will present some of our recent work in atomistic and coarse-grained simulations and continuum modeling for this problem. Application of these methods in the design of ocular drug delivery systems and novel packaging materials will also be discussed.



Self-assembly behavior of bottlebrush copolymers in solution: From molecular dynamics to machine learning

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Abstract

The investigation of bottlebrush copolymer self-assembly in solution involves a comprehensive approach integrating simulation and experimental research, due to their unique physical characteristics. However, the intricate architecture of bottlebrush copolymers and the diverse solvent conditions introduce a wide range of parameter spaces. In this study, we investigated the solution self-assembly behavior of bottlebrush copolymers by combining dissipative particle dynamics (DPD) simulation results and machine learning (ML) including graph convolutional networks (GCNs). The architecture of bottlebrush copolymers is encoded by graphs including connectivity, side chain length, bead types, and interaction parameters of DPD simulation. Using GCN, we accurately predicted the single chain properties of bottlebrush copolymers with over 95% accuracy. Furthermore, phase behavior was precisely predicted using these single chain properties. Shapley additive explanations (SHAP) values of single chain properties to the various self-assembly morphologies were calculated to investigate the correlation between single chain properties and morphologies. In addition, we analyzed single chain properties and phase behavior as a function of DPD interaction parameters, extracting relevant physical properties for vesicle morphology formation. This work paves the way for tailored design in solution of self-assembled nanostructures of bottlebrush copolymers, offering a GCN framework for precise prediction of self-assembly morphologies under various chain architectures and solvent conditions..^[1]

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DNA Condensation and Aggregation Induced by Charged Agents

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Abstract

While DNA is one of the longest and the stiffest molecules in nature and is negatively charged, they are strongly condensed in a tiny space of cell nuclei and in some virus thanks to polyvalent cations and/or small basic proteins. For example, protamine, a small arginine-rich basic protein plays an important role in packaging paternal genome into sperm nuclei during spermatogenesis, achieving a 10^6 -fold compaction of DNA, corresponding to a 10-20 times higher compaction than in somatic cells. The microscopic mechanism at play and the resulting DNA organization are not yet fully understood.

Using molecular modeling, we investigate the condensation of dsDNA chains (up to 8000 bp) and the aggregation of short dsDNA fragments (50 to 150 bp) driven by biological-relevant condensing agents: a short polyamine (spermine 4+) and a strongly basic and internally disordered protein (salmon protamine +21). Idealized models for dsDNA (roughly reproducing grooves), polyamine and protein, incorporating solely long-range electrostatic with explicit ions and steric interactions are used to capture and highlight generic behaviors in semi-dilute solutions and in confined geometry. Induced DNA morphologies are explored as a function of the short / long polycation and nucleic acid charge ratio and relevance to microscopic organization in bacteriophage and in sperm nucleus is discussed.

Molecular Dynamics Simulation of Compression-Induced Fracture in Polymer Nanoparticles

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Abstract

Small particles made of organic and inorganic materials are used in a wide range of applications, from everyday products to advanced fields. Their mechanical properties, such as elastic modulus and elastic–plastic deformation behavior, strongly affect material performance and reliability. These properties have been evaluated using flat-plate compression tests, which allow individual particles to be deformed to high strains. Previous tests on polystyrene and acrylic polymer particles have yielded stress–strain curves that differ from those of the corresponding bulk materials. However, it remains unclear whether these differences arise from miniaturization or simply from particle geometry. Understanding the mechanical and fracture behavior of nanoparticles is challenging because their curved surfaces lead to nonuniform deformation. Although several models, including the Hertz, Abbott–Firestone, and Kogut–Etsion models, have been proposed, they rely on simplifying assumptions or continuum mechanics and cannot describe molecular-scale fracture processes within nanoparticles. Therefore, in this study, we used all-atom molecular dynamics simulations to clarify the molecular-scale mechanisms underlying the compression-induced deformation and fracture of polymer nanoparticles. We investigated poly(methyl methacrylate) (PMMA) and poly(methyl acrylate) (PMA), which have similar chemical structures but different glass transition temperatures.

Using the applied load, F , and the nanoparticle radius before compression, r_0 , we calculated the engineering stress as $\sigma_{\text{eng}} = F/(\pi r_0^2)$. Consistent with previous compression tests on polymer nanoparticles, σ_{eng} exhibited an S -shaped curve, suggesting rubber-like mechanical behavior even for glassy polymer nanoparticles. We therefore calculated the true stress as $\sigma_{\text{true}} = F/A(\varepsilon)$, where $A(\varepsilon)$ is the actual contact area determined from the number of plate atoms experiencing repulsive interactions with the nanoparticle. The contact area increased linearly in the elastic region, consistent with Hertz theory, and deviated from this trend at larger displacements $d > 5$ nm. For PMMA, σ_{true} exhibited yielding near $d = 5$ nm, strain softening near $d = 10$ nm, and strain hardening near $d = 18$ nm, consistent with the behavior of bulk PMMA. In contrast, PMA, which has a lower T_g , did not exhibit clear yielding. Thus, true stress enables the mechanical behavior of polymer nanoparticles to be discussed on the same basis as that of bulk polymers and reproduces the differences between PMMA and PMA. [1] Takahashi I. et al., *ACS Appl. Nano Mater.* **2025**, 8, 9276–9285.

Tailoring catalysts for reactions involving multifunctional molecules using machine learning

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Abstract

First principles methods and more recently machine learning, have opened new avenues to systematize catalyst design. Yet, computational efforts of the last 2+ decades have primarily focused on reactions involving small molecules (C_{1-2} , O_1 , N_1) that are activated by high-symmetry sites of extended surfaces at low surface coverages. In contrast, most industrial processes involve large multi-functional molecules (e.g., cyclic hydrocarbons, nitroarenes, lignin-derived molecules etc.) that are activated by low-symmetry sites of nanoclusters under high surface coverages. Machine learning methods have emerged as a powerful approach to bridge this gap between first principles models and reality. Using physics-inspired machine learning trained on small datasets by active learning, we identify next-generation bimetallic Pt catalysts for dehydrogenating liquid organic hydrogen carriers like methylcyclohexane. Using machine learned potentials, we rationalize why functionalized nitroarenes adsorb in self-assembled monolayer-like arrangements on Pd catalysts, consistent with in situ surface characterization. We distil our learnings into best practices for using vanilla/minimally-trained machine learned potentials to predict the surface structure and reactivity of multi-functional molecules on low symmetry catalytic surfaces.

Insights into CO dimerization at electrified Cu interfaces from large scale machine learning simulations

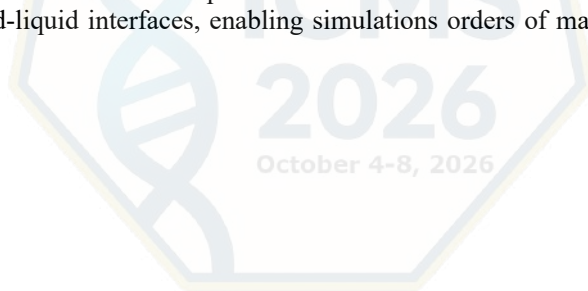
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Abstract

Catalysis at solid-liquid interfaces underpins many energy technologies, yet ab initio simulations that capture interfacial dynamics remain prohibitively expensive. Here we introduce Open Catalyst 2025 (OC25), the largest dataset for solid-liquid interfaces. To demonstrate OC25-trained models as practical tools for electrocatalysis, we investigate CO dimerization on Cu surfaces, a key step in CO electroreduction. Using large cells (>800 atoms) and enhanced sampling up to 7 ns - the largest explicit-solvent CO dimerization study to date - we compute free-energy profiles under varied surface charge, cation identity, and surface facet. We find that dimerization is weakly sensitive to charge and cation identity, with appreciable stabilization only at the most negative charge densities, while extension to stepped Cu(310) reveals a more favourable pathway at modest reducing potentials. Our results demonstrate that OC25-trained models provide a scalable tool for investigating electrocatalytic transformations at solid-liquid interfaces, enabling simulations orders of magnitude beyond ab initio methods.



Reactive Molecular Simulations of Catalytic Surfaces and Solid–Liquid Interfaces Using Neural Network Potentials

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Abstract

Neural network potentials (NNPs) provide a powerful approach for extending first-principles molecular simulations to complex catalytic surfaces and solid–liquid interfaces. In this talk, I will present recent developments in our group in NNP-based molecular simulations for understanding interfacial reaction dynamics and adsorption thermodynamics under finite-temperature and finite-pressure conditions.

First, I will discuss NNP-based molecular dynamics simulations of water and alcohol interfaces with metal oxides such as CeO₂ and ZrO₂.^[1–3] Nanosecond-scale simulations reveal surface hydroxylation equilibria, proton hopping, ion transport, and facet-dependent adsorption and dissociation dynamics that are difficult to access by conventional DFT-based molecular dynamics. Second, I will introduce NNP-coupled grand canonical Monte Carlo simulations for hydrogen adsorption on metal surfaces. Applications to Pt, Pd, Ir, and stepped Pt surfaces clarify coverage-dependent site preferences, hydrogen–hydrogen interactions, and adsorbate-induced surface restructuring.^[4–6] In particular, simulations of Pt(533) and Pt(553) show that high hydrogen chemical potentials can induce step-edge roughening, indicating that active surface morphology may depend on the reaction environment.

These examples demonstrate how NNP-based simulations can bridge first-principles accuracy and statistical sampling, providing molecular-level insight into reactive interfaces under realistic catalytic conditions.

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Breakage in Wetting Transparency: A Molecular Insight

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Abstract

Liquids interacting with chemically or physically distinct surfaces exhibit diverse wetting behaviour governed by interfacial tensions and commonly described in terms of solvophilicity and solvophobicity. Wettability on an ideal, rigid, flat substrate is traditionally quantified by the contact angle. However, the contact angle is inherently droplet-size-dependent due to line-tension effects and becomes increasingly ambiguous in complex wetting situations^[1] involving variation in lattice planes, surface roughness, chemical heterogeneity, curvature, and substrate deformability. Furthermore, fluid imbibition into rigid or soft porous substrates can significantly alter apparent wetting behaviour, particularly at electrochemical interfaces. These limitations call for a universal, molecularly grounded definition of wettability applicable to both non-deformable and deformable soft surfaces. Here, we propose a droplet-size-independent framework in which wettability emerges from the intrinsic coupling between molecular ordering and mobility within the contact plane. Using molecular dynamics (MD) simulations, we demonstrate that liquid molecules at the contact plane undergo a surface-directed phase transition as liquid-solid adhesion increases. This transition is quantified through in-plane excess-entropy-diffusivity scaling: solvophobic surfaces exhibit bulk liquid-like, low-order, high-diffusivity interfacial behaviour, whereas solvophilic surfaces display highly ordered, low-mobility, solid-like interfacial layers. The proposed excess-entropy-diffusivity-wettability framework^[2] consistently captures anomalous wetting transitions arising from variations in adhesion strength, surface lattice structure, and roughness on rigid substrates. For porous substrates, it quantitatively accounts for the influence of fluid imbibition on overall spreading behaviour. For deformable substrates, the framework also incorporates surface softness via interfacial molecular structure, enabling the prediction of wetting transitions without relying solely on macroscopic geometric measures. In the aforementioned fashion, this framework establishes a unified basis for understanding complex wetting phenomena beyond conventional contact-angle descriptions.

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Catalytic conversion of CO₂ and CH₄ into acetic acid and formic acid through Ni₁₃ clusters supported on MgO surface : A DFT study

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Abstract

Catalytic conversion of CO₂ and CH₄ to obtain essential chemicals is a promising way of utilizing carbon resources to diminish CO₂ emissions and to mitigate global warming. For the catalytic conversion, metal catalyst plays a commendable role in the catalytic activity with the good activation capabilities. In this regard, nickel clusters gain huge attention with prominent catalytic activity and higher natural abundance. Our computational investigation performed through density functional theory calculations provides the possible reaction pathways to obtain acetic acid and formic acid by catalytic conversion of CO₂ and CH₄ gases through Ni₁₃ clusters and MgO surfaces. Our results evidence the strong adsorption of CO₂, CH₄ and their intermediates on the Ni₁₃ clusters deposited on the MgO surface. Our work also witnessed the oxidized Ni₁₃ clusters are more stable and prominent for the catalytic activity. On MgO thin films supported on Ag, thermodynamically favorable reverse oxygen spill over facilitates the oxidation of Ni₁₃ clusters through excess oxygens trapped between the Ag(100) and MgO surfaces. Catalytic conversion reactions carried out on the oxidized Ni₁₃ clusters placed on the MgO and Ag(100) surface also exhibit prominent adsorption and validates the reactions pathways in both unoxidized and oxidized Ni₁₃ clusters.

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Beyond the Bead-Spring: Emergent Physics in Crowded, Charged, and Topologically Constrained Polymer Systems

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Abstract

Coarse-grained polymer models, often reduced to little more than excluded volume, connectivity, and a handful of effective interactions, continue to reveal physics far richer than their minimal ingredient lists would suggest. In this talk, I will draw on three distinct lines of work from our group to illustrate this point. First, in neutral polymers immersed in crowded environments, the size, density, and attraction strength of crowders act as three architectural control parameters that reshape the polymer's phase diagram, drive reentrant coil-globule behavior, and extend naturally to multi-chain aggregation. Second, in charged polymers, we have extensively studied how counterion condensation drives the collapse and aggregation of inherently like-charged chains, despite the underlying electrostatic repulsion; building on this foundation, we then examine how crowder bridging competes with and modifies counterion-mediated condensation, adding a further layer of complexity absent in neutral systems. Third, ring polymers, through their closed-loop topology alone, give rise to topological glasses governed by inter-ring threading, with stiffness and composition controlling a melting-to-stacking transition into ordered columnar phases. Together, these three systems show how a common coarse-grained modeling philosophy, applied to different molecular architectures, uncovers a strikingly diverse landscape of collapse, aggregation, and glassy phenomena.

Membrane Organization and Remodeling Revealed by SPICA Coarse-Grained Simulations

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Lipid membranes are dynamic molecular platforms that regulate intracellular delivery, cellular signaling, and viral assembly. Their functions arise from complex coupling among lipid composition, molecular shape, electrostatics, membrane stress, curvature, and protein–lipid interactions. This presentation highlights recent applications of the SPICA coarse-grained force field^[1] to biologically important membrane systems, demonstrating how molecular simulations can reveal physical principles underlying membrane organization and remodeling.

The first example concerns the endosomal escape of lipid nanoparticles (LNPs), a major bottleneck in gene delivery. Simulations of pH-sensitive amino-lipid-containing LNPs interacting with model endosomal membranes show that protonated ionizable lipids promote membrane fusion through electrostatic interactions with anionic endosomal lipids. Lipid transfer, stalk formation, and subsequent pore expansion provide a molecular pathway for nucleic-acid release. These results suggest that lipid shape, pH-dependent charge regulation, membrane tension, and payload localization are key determinants of endosomal escape efficiency.^[2]

The second example addresses asymmetric plasma membranes based on lipidomic data. Cholesterol preferentially partitions toward the outer leaflet, generating differential lateral stress: compression in the outer leaflet and tension in the inner leaflet. This stress enhances leaflet-specific properties, producing a tightly packed, ordered outer leaflet and a more fluid inner leaflet with dynamic nanoscale domains. Comparison with scrambled membranes suggests that lipid asymmetry limits domain growth and helps maintain nanoscale membrane heterogeneity.^[3]

The final example focuses on SARS-CoV-2 envelope assembly. By systematically varying viral protein composition, lipid composition, and protein orientation, the simulations show that stable envelope formation with the correct topology requires synergistic matrix–spike protein interactions together with specific protein–lipid interactions in heterogeneous ERGIC-like membranes.^[4]

Together, these studies illustrate how SPICA simulations link molecular interactions to mesoscopic membrane behavior, offering mechanistic insight into lipid-based nanomedicine, plasma membrane organization, and viral envelope formation.

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Methods for simulating coarse-grained structure-based models of biomolecules.

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I will present three parts which aid molecular dynamics (MD) simulations of coarse-grained structure-based models of biomolecules: (1) A software toolkit that generates input files to simulate such force-fields within standard simulation packages such as OpenSMOG/OpenMM and Gromacs; (2) A method for increasing the sampling efficiency of coarse-grained models of biomolecules; (3) A form of potential which helps with the MD simulations of 3D-domain-swapping in proteins.



Enzyme Catalysis and Free Energy Landscapes

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Abstract

The thermodynamics and kinetics unique to the catalytic behavior of enzymes are encoded within the metastable states, separated by barriers, in the underlying free energy landscape.^[1] However, construction and interpretation of such landscapes in biomolecular systems is challenging on account of an inherently high dimension. In this lecture, we highlight how classical unbiased and accelerated molecular dynamics simulations may be used to partition the high dimensional conformational space of any enzyme in to sub-states with the aid of Markov state models and derive the transition network between different functionally relevant conformations. We also demonstrate how the full free energy landscape may be derived in terms of free energy disconnectivity graphs. The application of these methods will be discussed to understand the effect of pH,^[2] dimerization^[3] and glycosylation^[4,5] on the functional dynamics of the enzyme human carbonic anhydrase II.

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October 4-8, 2026

SketchDNA: A GUI-Enabled Toolkit for Multiscale Modeling of Topological DNA Structures

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Abstract

Computational modeling tools have enabled detailed exploration of the structural dynamics of nucleic acids at the nanoscale. Despite these developments, a unified platform for creating multiscale models of topological DNA structures, which are of fundamental importance across rapidly converging biological disciplines, is lacking. In this talk, I will introduce a GUI-enabled topological DNA design tool, SketchDNA (SDNA), that facilitates a user-friendly interface to create all-atom (AA) and coarse-grained (CG) models of DNA structures with tunable topological parameters. Building on the modular and open-source framework of SDNA, the software can be readily integrated with both emerging and existing DNA design platforms, such as oxDNA, MrDNA, etc. I will demonstrate the utility of SDNA computational framework by illustrating the conformational dynamics of three representative topological DNA structures, minicircles, catenanes, and Borromean rings. Analyzing AA and CG molecular dynamics (MD) simulations of these topological DNA systems using the AMBER and Martini DNA force fields, respectively, we have characterized their equilibrium structural dynamics, fluctuations, and topological properties. While the AA simulations allow us to characterize the topology-dependent structural rearrangements at the nucleotide level, long-timescale CG simulations reveal supercoiling-induced conformational transitions. The multiscale SDNA toolkit broadens the applications of MD simulations by enabling in-situ characterization of the biophysical properties of topological DNA nanostructures. The GUI version of SDNA is available at <https://sdna.biotech.iith.ac.in>, while the source code is accessible at GitHub^[1]

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Curcumin-Gold Nanocomposites for Enhanced Doxorubicin Delivery: Molecular Mechanisms of Loading and Membrane Interactions

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Abstract

Curcumin-functionalized gold nanoclusters are promising platforms for catalysis and drug delivery, yet the molecular determinants of their stability, morphology, and solvent response remain unclear. Here, microsecond all-atom molecular dynamics simulations are employed to investigate a 2 nm gold nanoparticle noncovalently coated with different curcumin forms, including neutral enol and trans-keto tautomers, the deprotonated enolate, and their mixtures in water-ethanol and water-methanol solvents. Layer-resolved analyses of radius of gyration, density profiles, and surface coverage reveal that neutral enol and trans forms generate compact assemblies with near-complete surface coverage, whereas enolate-rich systems adopt more expanded conformations with solvent-exposed molecules. Mixed systems preserve these intrinsic packing characteristics while improving overall coverage. Solvent substitution from ethanol to methanol reduces π - π stacking, strengthens Au-curcumin interactions, and increases surface coverage, yielding more nanostructures that are compact. Free energy and potential of mean force calculations indicate that deprotonated curcumin most effectively screens Au-Au interactions and stabilizes dispersed nanoparticles, while neutral tautomers provide moderate stabilization. Curcumin also enhances the loading of anticancer drug doxorubicin (DOX) onto Au nanoparticles, improving biocompatibility. Enolate(An)-containing systems produce extended structures with weaker membrane interactions, whereas neutral curcumin complexes form compact, positively charged assemblies that strongly bind to negatively charged cancer cell membranes. These findings clarify how tautomeric state and solvent environment cooperatively govern interfacial organization and colloidal stability; establish design guidelines for curcumin-based gold nanocarriers in catalysis, sensing, and drug delivery applications.

Keywords: Curcumin, gold nanoparticle, doxorubicin, nanocomposite, cancer drug delivery, cell membrane, potential of mean force (PMF), solvent conditions.

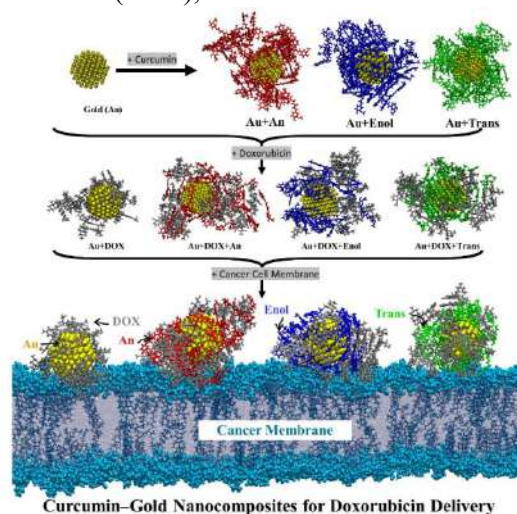


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Ultralow nanofriction phenomenon on articular cartilage interfaces: Insights from atomistic simulations

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Abstract

Articular cartilages exhibit superior lubricating properties at multiple scales (friction coefficient COF 0.0005-0.04) throughout millions of articulation cycles [1]. The nanoscale contact interface behavior is highly influenced by the constitution, structural arrangement of macromolecules, loading, shear rates, hydration, ionic concentration within soft confinements [2]. This unique lowering of friction at the cartilage-synovial interfaces is attributed to the synergistic molecular level interactions of various macromolecules present at the interface such as collagen, aggrecan, hyaluronan, and lubricin from the synovial fluid which act under severe physiological loading and shearing conditions [3]. Although the physics of boundary lubrication at the cartilage interfaces have been investigated at nanoscales, still there is a lack of deeper understanding of evolution of uniquely ultralow friction mechanisms from an atomistic perspective. In this work, classical non-equilibrium molecular simulations are conducted on developed articular cartilage-cartilage top layer contact atomistic models and systematically investigated for their nanoscale tribological properties such as contact, adhesion, and frictional behavior under varied loads and sliding speeds to interpret the physiological shearing phenomenon. Nanomechanical tests for dependence of friction on various parameters such as load, interface hydration, sliding speeds, ionic content on these idealized cartilage models revealed underlying small-scale boundary lubrication phenomenon which are not accessible through experimental characterization techniques. Articular cartilage at high loading and varying shear rates, provides ultralow frictional properties COF in the range of 0.0015-0.027 employing water molecules with various combinations of ions resisting shear deformation. In comparison, unhydrated cartilage interfaces exhibit heavy deformation and delamination due to molecular entanglement and stretching offering COF in the range of 0.2-0.75 which was found to be in good agreement with previous experimental investigations in literature conducted on top layer cartilage constituents. Water movement within soft confined environment, protein side chains dynamics, shear rates play a major role in lubricating these tissue interfaces. Overall, this work provides atomistic insights of underlying mechanisms of nanoscale friction and cartilage interface failure which have implications in developing smart biomimetic surface solutions.

Keywords: Articular Cartilage, Biolubrication, Molecular simulations, Nanomechanics.

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Toward the exact exchange-correlation functional: A neural network construct

GuanHua Chen^{1,2*}

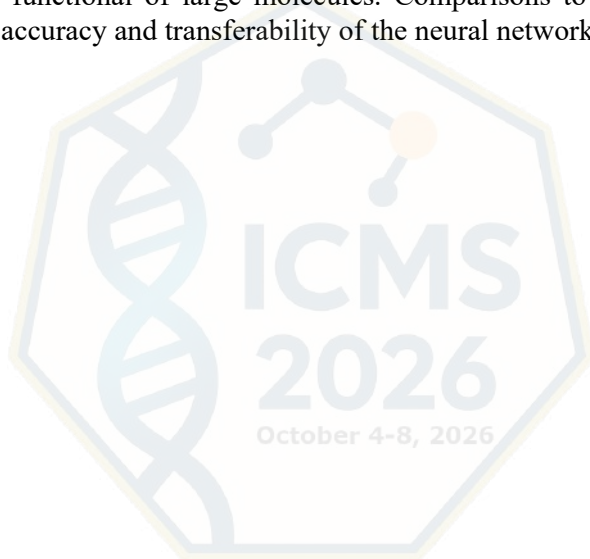
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Abstract

Deep neural network can be employed to construct exchange-correlation functional. It requires merely the electron densities of small molecules and ions and yet can determine the exchange–correlation functional of large molecules. Comparisons to B3LYP and PBE are given to illustrate the accuracy and transferability of the neural network based XC functional.



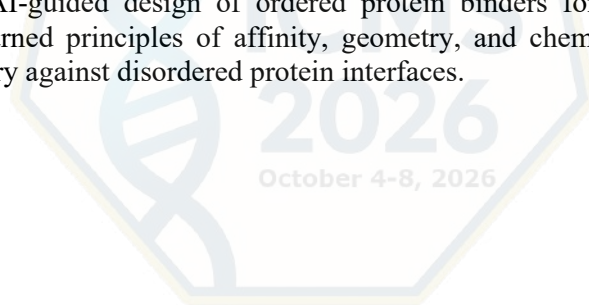
AI-Guided Prediction and Design of IDR–Protein Interactions

Subinoy Adhikari, Soham Choudhuri, **Jagannath Mondal***

Tata Institute of Fundamental Research Hyderabad's affiliation and full address in 10-point size Times New Roman font, centered, italicized.

Abstract

Intrinsically disordered regions (IDRs) mediate many regulatory protein interactions but remain difficult to model because of their heterogeneous conformations, context-dependent recognition, and poorly defined binding interfaces. In this talk, I will present our data-driven and machine-learning efforts to quantify and design IDR–protein interactions. First, I will introduce **IBPC-(K_d)**, a curated dataset of 1,785 IDR–ordered protein complexes with experimentally measured binding affinities, spanning more than six orders of magnitude. Analysis of this dataset reveals shape complementarity, partner-surface order, and electrostatic asymmetry as major determinants of IDR binding strength. Building on these insights, we developed **IDRBindNet**, a graph-transformer model that combines protein language model embeddings, interface geometry, and residue-level chemical context to predict dissociation constants with state-of-the-art accuracy. I will also discuss our ongoing extension of this framework toward AI-guided design of ordered protein binders for a given IDR target, highlighting how learned principles of affinity, geometry, and chemical compatibility can support drug discovery against disordered protein interfaces.



DFT-ML guided design of bimetallic nanoparticles for methane activation

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Abstract

Methane (CH₄) a primary constituent of natural and shale gas can be converted into syngas via partial oxidation, steam reforming and dry reforming reactions. This syngas serves as a versatile intermediate to produce various value added chemicals and fuels. For most of these methane conversion reactions, methane activation is the rate-determining step^{1,2}. Transition metal nanoparticles have emerged as promising catalysts capable of lowering this activation barrier and enabling methane conversion at low temperature³. In this study machine learning models are used to predict activation energies for methane dissociation on bimetallic nanoparticles. At first by using DFT simulations activation energies for methane activation were calculated on different Pt nanoparticles of varying shapes (Truncated Octahedral (TO), Regular Truncated Octahedral, Cuboctahedral and Octahedral) and sizes. Out of these TO₃₈ nanoparticle were observed to exhibit least activation energy for methane dissociation and was chosen as a suitable model for further calculations. ML model were build using a dataset comprising of 110 DFT-calculated activation energies for methane C–H bond cleavage on TO₃₈ transition metal based bimetallic nanoparticles wherein FCC transition metal served as the base metals and were alloyed with other transition metals and post transition metals consisting of A₃B and AB-type alloy composition. Among all the models tested, the random forest regressor model showed the best performance with the root mean square errors (RMSEs) of 0.19 eV for predicting CH₄ activation barrier on bimetallic nanoparticles. Further multi-objective optimization was systematically performed to identify optimal bimetallic catalysts by explicitly tuning the relative importance of activity, cost and sustainability descriptor within a unified screening framework. Cu₃Co and CuMn were identified as optimal candidates, reflecting strong sustainability characteristics along with reasonable activity.

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Designing transferable collective variable and accelerating sampling in bio-molecular systems using explainable AI

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Choosing appropriate collective variable for bio-molecular processes is a challenging task. Moreover, while constructing the free energy landscape of flexible biomolecules, solvent degree of freedom is often neglected to reduce the computational burden. Thus, we have intentionally included the first hydration layer water molecules as a collective variable in the optimized CV framework to systematically quantify the contribution of water in different biophysical systems with varying complexity. Moreover, in our previous work, we have proposed one protocol to quantitatively identify the contribution of different OPs locally in the transition state ensembles (TSE) through XGBoost model with explainable AI algorithm Shapley Additive exPlanation (SHAP). Using this protocol, we have shown that hydration water is the most crucial order parameter which dictates the major barrier for polymer collapse transition. We further extend this protocol to find out the optimized slowest coordinate in protein folding transition. We have developed a neural network architecture based on autoencoder framework with time-lag information to accurately capture the system's kinetics and denoising framework which can reduce the noise present in the data to separate multiple low populated metastable basins present in the free energy landscape. We have chosen three systems: a mutant of chignolin, Trp-cage-wild type and a mutant of trp-cage and shown that our method identified multiple metastable basins in the landscape. We have also found folding and unfolding times calculated from MSM shows close resembles with the experiments. Moreover, using the proposed protocol of analyzing contribution of OPs in the TSE, we have found that hydration water represents the major barrier for this system which essentially means that desolvation of water molecules from the hydrophobic core of these two proteins is the slowest step.

Next, we have developed an enhanced sampling method combining metadynamics with an interpretable AI model. We have shown that incorporating transition state ensembles knowledge in doing well-tempered metadynamics drastically improves the sampling in these polymer systems and achieve faster convergence in free energy profiles. We have also shown the application of this enhanced sampling method in two protein-ligand binding systems (Hydrophobic cavity-ligand and T4 lysozyme) where it shows faster free energy surface exploration within just 200 ns. Overall, our framework is general enough to analyze different OPs contribution in TSE from long unbiased simulation and also performing enhanced sampling with this.

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From Trajectories to Narratives: Autonomous Multimodal Reasoning in Computational Chemistry with EyeCue

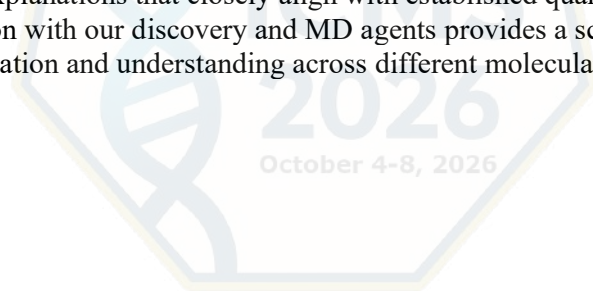
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Abstract

Scientific workflows are now increasingly made to work with AI agents to automate complex analyses. Yet, communicating results in an intuitive and explainable manner remains a challenge. We present EyeCue, a multimodal framework that can be integrated with AI agents to automatically generate narrated visual analyses and concise summaries from scientific analysis. EyeCue combined with agents capable of multimodal reasoning, domain knowledge, and natural language generation helps transform complex computational results into human-interpretable video narratives that highlight key observations and insights. As a representative application, EyeCue analyzes molecular dynamics simulation trajectories to identify events such as binding sites, protein ligand interactions, conformational changes, producing narrated explanations that closely align with established quantitative analyses. EyeCue in conjugation with our discovery and MD agents provides a scalable approach for enhancing communication and understanding across different molecular systems.



Decoding Clade-Specific bNAb/HIV-1 Env Interactions Using Machine Learning

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Abstract

Human immunodeficiency virus type-1 (HIV-1) exhibits extraordinary genetic diversity at a global scale, and this extensive variability remains a fundamental challenge for the development of an effective AIDS vaccine. Individuals infected with HIV-1 can develop broadly neutralizing antibodies (bNAbs), which provide critical insights for the design of vaccines aimed at broader global protection. The structural and energetic descriptors were extracted from the 3D structural data (PDBs) of the protein-protein complexes. In this study, machine-learning approaches were employed to predict the binding free energies or affinities (ΔG , kcal/mol or K_D , nM) of bNAbs across different HIV-1 clades (subtypes)^[1-3]. An extreme gradient boosting (XGBoost) regression model was developed and demonstrated superior performance compared to other regression models, achieving a training R^2 of 0.92 and a test R^2 of 0.658. The predicted ΔG values reveal consistent clade-dependent binding patterns, particularly within clade B, whereas clade G exhibits disproportionate behavior in regions associated with reduced neutralization potency. The predicted binding free energies (ΔG) follow the trend: gp120-gp41 interface $\approx$ fusion domain $>$ CD4 binding site (CD4bs) $>$ V1V2 loop $\approx$ V3-glycan. This trend is broadly consistent with experimentally reported binding affinities of benchmark bNAbs within each epitope class. Clade C bNAbs-Env pairs occupy an intermediate position in terms of neutralization potency. While some bNAbs, such as 3BNC117, VRC01, and 10-1074, retain strong activity with potent IC50 values, others, including PG9 and 2G12, exhibit substantially reduced potency. This heterogeneous behavior is consistent with the well-established susceptibility profile of clade C isolates. Overall, the study provides quantitative insights into clade-dependent bNAb binding energetics and highlights the utility of machine learning for guiding HIV-1 immunogen and vaccine design.

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PEDOT:PSS Stretchability Enhancement Induced by Hard-Cation-Soft-Anion Ionic Liquids: Simulated Mixing, Drying, Pulling, and Scale Bridging

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Abstract

PEDOT:PSS is a promising material for electronic-skin applications but it still exhibits limited conductivity and stretchability. Vigorous mixing with hard-cation-soft-anion ionic liquids (ILs) has emerged as a powerful tool to enhance its conductivity.^[1-7] Recent experiments have demonstrated that such IL treatments improve its stretchability as well,^[6] but the molecular mechanism behind such enhancements remains unclear. Herein we use molecular dynamics simulations to investigate structural and mechanical effects of treating PEDOT:PSS with two hard-cation-soft-anion ILs such as 1-ethyl-3-methylimidazolium and 3-methylimidazolium tetracyanoborates. Starting from the simulations on the aqueous solution models of pristine and IL-treated PEDOT:PSS (simulated mixing), we mimic water evaporation at various temperatures (simulated drying and annealing up to 140°C). The resulting fibular structure of PEDOT:PSS is then subjected to uniaxial deformation to mimic the stress-strain curves (simulated pulling). This series of simulations reveal that the IL treatment indeed reduces the elastic modulus and the maximum stress of PEDOT:PSS, agreeing with the experimental findings. Hydrophilic (hard) cations, such as the protic 3-methylimidazolium, indeed plays a critical role in this improvement by holding water around them in the dry film. This is a showcase where IL-induced rearrangements at the molecular level translate into improved macroscopic stretchability and mechanical robustness. Such molecular-level insights would provide a foundation to develop intrinsically stretchable conducting polymer films and pave a way for their application in stretchable electronic devices. To draw more realistic picture of the materials and processes at a larger scale, we are now developing a coarse-grained model of PEDOT:PSS from the above atomistic simulation data, utilizing AI for the scale bridging.

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Decoding Hotspots within Perturbed Protein Systems: Learning from Data and Networks

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Abstract

Complex biomolecules often do not yield easily to standard biophysical evaluations. Large scale ensemble data typically obscure subtle signatures of perturbation response, or evolutionary progression. These pose major challenges not just to experiments, but to *in silico* thermodynamic sampling. In this presentation, we first discuss our simple, but interpretable supervised machine learning approach for developing an importance (or sensitivity) index to pressure-induced perturbation in a folded protein. While the overall rigidity landscape of the protein shows only modest pressure dependence, top-ranked residues exhibit pronounced, pressure-specific alterations in solvent association. In the case of enzymes such as kinases, information entropy-based approaches showcase the hotspots whose mutational changes correlate with alterations to activity. Finally, we show how deep neural networks offer can be employed as a plausible route for predicting biological manifestations such as protein-induced membrane curvature change.

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Understanding Gas Sensing through Multiscale Simulations of Impurity-Modulated Charge Transport

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Abstract

Organic semiconductor gas sensors are promising for agriculture, environmental monitoring, and medical diagnostics because they enable low-power, room-temperature operation on low-cost and mechanically flexible platforms. Several mechanisms have been proposed for organic NH₃ sensors, including H₂O-assisted de-doping, direct modulation of charge transport, and receptor-mediated Lewis acid–base interactions,^{[1],[2]} which may coexist within a device. Recent experiments by our collaborators showed that CzDBA, a boron-containing anthracene derivative, exhibits ultralow NH₃ detection limits and high sensitivity. Motivated by the Lewis acidity of its boron centers, we use multiscale simulations to investigate how B···NH₃ binding perturbs the electronic structure and reduces charge-carrier mobility.

Our framework combines density functional theory, molecular dynamics, and kinetic Monte Carlo simulations within a hopping-transport model.^[3] We first evaluate sequential NH₃ adsorption because each CzDBA molecule contains two boron centers. The adsorption free energy of the first NH₃ molecule is approximately −0.02 eV, indicating weak but favorable binding consistent with the experimentally observed reversibility after removal of the NH₃ source. In contrast, adsorption of a second NH₃ molecule is unfavorable, with a free energy above 0.15 eV. Thus, each CzDBA molecule is expected to bind at most one NH₃ molecule under the sensing conditions.

We then construct amorphous CzDBA models containing 0–1% NH₃-bound complexes and evaluate their hole-transport properties. The simulated hole mobility decreases systematically with increasing NH₃–CzDBA concentration. This reduction is dominated by charge trapping: the NH₃–CzDBA complex has a more favorable hole site energy than pristine CzDBA, causing holes to localize on the bound species. Its slightly larger hole-transfer reorganization energy provides an additional, but smaller, contribution. Overall, this work identifies Lewis acid–base binding between NH₃ and boron-containing semiconductors as an additional sensing mechanism. The results provide design principles for high-performance gas-sensing materials and a general computational framework for connecting molecular binding events with macroscopic sensor responses.

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Sequence-Specific Folding and Collective Organization of Partially Active Polymers

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Abstract

Biological polymers are driven out of equilibrium by localized processes such as ATP/GTP hydrolysis, motor activity, and enzymatic remodeling, which generate spatially heterogeneous forces along their contours. Similar heterogeneity can be engineered in synthetic polymers through catalytic, light-responsive, or chemically active units. Partially active polymers therefore provide minimal models for understanding how the spatial patterning of active forces controls macromolecular folding and collective organization, with potential relevance to biomimetic and reconfigurable soft materials.

Using Brownian dynamics simulations, we investigate self-avoiding polymers containing active Ornstein-Uhlenbeck monomers arranged in different sequences along the chain. We first examine the folding of a single partially active polymer and compare dry dynamics with simulations incorporating hydrodynamic interactions. We find that activity patterning can drive pronounced sequence-dependent coil-to-globule transitions, although the passive polymer remains swollen under the same conditions. The collapse is accompanied by active-passive segregation and a reduction in swim pressure, linking the spatial arrangement of activity directly to the folded state. Hydrodynamic interactions modify the steady-state conformations, shift the collapse boundary, alter internal monomer relaxation, and produce deviations from conventional Zimm-like behavior. We then extend this framework to multichain systems and uncover sequence-dependent reentrant phase behavior controlled by activity and polymer density. Sequences with intermediate blockiness phase separate above a critical density within an intermediate activity window, whereas well-mixed sequences remain largely coil-like and sufficiently high activity restores a homogeneous state. These results suggest that sequence-dependent chain compaction and the associated suppression of swim pressure provide a microscopic route to activity-induced phase separation. Together, this work identifies activity patterning and hydrodynamic coupling as nonequilibrium control parameters for the folding and assembly of active macromolecules.

Molecular Origin of Self-Organized Nematics

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Abstract

Nematic liquid crystals (NLCs) are attractive candidates for next-generation sensing, photonic, and optoelectronic applications owing to their responsiveness to external stimuli, arising from molecular anisotropy. However, achieving self-organized nano/micropatterns in thin NLC films is a longstanding challenge due to anisotropic orientation-driven elastic constraints, which often suppress spontaneous instability growth and morphological evolution at room temperature. In this work, we demonstrate how two common non-invasive routes – solvent evaporation technique and electrohydrodynamic (EHD) patterning, can be utilized to generate on-demand self-organized patterns in thin NLC films. Through atomistic molecular dynamics (MD) simulations, we show that solvent molecules fundamentally alter the intermolecular interaction landscape, generating entropic driving forces that produce concurrent changes in thermodynamic, dynamic, and rheological properties of the film.^[1] These molecular-scale transformations trigger instabilities, driving the emergence of diverse self-organized morphologies that are inaccessible in pure NLC films. Similarly, external electric fields alter molecular orientations, intermolecular energetics, and entropic landscapes, providing an additional mechanism for dictating instability, and morphological transitions. By tuning solute (NLC) concentration and electric-field strength, a rich spectrum of structures can be realized, including droplets, filaments, continuous films, hierarchical columnar morphologies in co-existence with secondary droplet-like features, and coalesced columnar networks, exhibiting intricate molecular orientations.^[1] Collectively, these findings reveal how intermolecular interactions orchestrate the coupling between molecular ordering, transport, and thermodynamic directionality, thereby dictating instability pathways and the emergence of complex self-organized morphologies in anisotropic thin films. These findings provide molecular design principles for tailoring self-organized morphologies in liquid-crystalline materials and other complex fluids, creating new opportunities for photomasks, optical templating, responsive sensing, and advanced nano/microfabrication technologies.

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Environment-specific flexibility assists polymer translocation

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Abstract

The translocation of polymers across membranes is an ubiquitous phenomenon in biological systems^{1,2}. Using two-dimensional Langevin dynamics, we investigate the translocation of a heteropolymer whose bending stiffness either remains fixed along the polymer backbone (sequence-specific stiffness, SSS) or adapts to the local cis-trans environment (medium-specific stiffness, MSS). We demonstrate that these two mechanisms lead to fundamentally striking contrast translocation dynamics. The SSS model exhibits pronounced mobility gradients, persistent tension build-up, anomalous sub diffusion, and enhanced dynamic heterogeneity arising from the coexistence of flexible and semiflexible domains. In contrast, adaptive flexibility in the MSS model dynamically homogenizes the chain, resulting in faster relaxation, smoother tension propagation, inhibited dynamic heterogeneity, and reduced ergodicity breaking. The evolution of the radius of gyration reveals strong stiffness-induced spreading in the SSS model, but a universal relaxation pathway once polymer stiffness adapts to the surrounding mediums in the MSS model. These results reveal how environmental modulation of polymer flexibility can govern translocation pathways and switching behaviour, offering design principles for tuneable transport in nanopore sensing, selective filtration, and biomolecular sequencing.

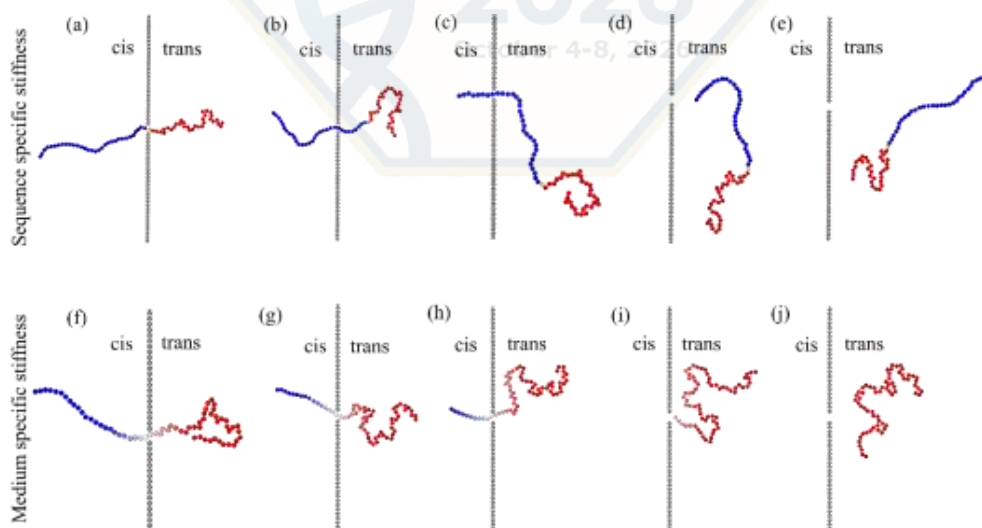


Fig 1. Schematic representation of the SSS model (a-e) and the MSS model (f-j), where the flexible (red) and semiflexible (blue) segments represents heterogeneity along the polymer backbone.

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Multiscale simulations of N-heterocyclic carbenes for the functionalization of metal surfaces

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Abstract

N-heterocyclic carbenes (NHCs) with suitable side groups exhibit the unique property of binding strongly to coinage metal surfaces via a single covalent bond whilst maintaining a high lateral mobility. Ab initio molecular dynamics simulations have revealed that the origin for this behaviour lies in the fact that such NHCs pull out a metal atom from the surface which then serves as a vehicle for NHC migration across the surface [1]. NHCs thus offer a promising alternative to thiol-based ligands for the formation of self-assembled monolayers.

For other applications, such as molecular rotors, it is desirable to anchor the NHCs at a fixed position on the surface. A unidirectionally rotating NHC species has been developed following theoretical design principles [2], for instance an asymmetric rotational potential as a prerequisite. By multiscale simulation, we demonstrate that this molecular motor can be driven by various forms of energy supply including temperature oscillations and inelastic electron tunneling from an STM tip.

Furthermore, we have shown that surface functionalization with NHCs can drastically enhance the catalytic properties of Pd nanoparticles. Density functional theory calculations predict a substantial lowering of activation barriers as a consequence of electron density being injected into the metal by the NHCs [3].

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Predicting Defect Topologies and Functionalization in 2D Materials and Their Effects on Nanoscale Transport

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Abstract

Defects, whether intentionally created or inadvertently formed, are ubiquitous in all materials. Nevertheless, not much is known about how these defects form in two-dimensional (2D) materials, what topologies of defects are more likely, and how defect topology affects the performance of 2D materials in various applications. In this talk, I will discuss the combined use of quantum-mechanical density functional theory (DFT) calculations, kinetic Monte Carlo (KMC) simulations, and chemical graph theory to predict nanopore shapes in graphene, hexagonal boron nitride (hBN), and molybdenum disulfide (MoS₂) in excellent agreement with transmission electron microscopy images. This will be achieved by the combination of DFT-derived etching energies of atoms, an experimentally calibrated etching energy–activation barrier relationship, stochastic simulations of atomic etching via KMC, and a graph-theoretic approach to compare nanopore shapes in 2D materials. Subsequently, I will discuss the development of a machine-learnable representation of nanopores, called STring Representation Of Nanopore Geometry (STRONG), to rapidly enumerate nanopores, determine unique functionalized topologies, and predict gas transport barriers. The prediction of gas transport barriers involves the use of a gated recurrent unit-based neural network architecture trained on molecular mechanics data. Moving forward, I will explain how defects influence water slippage on the surfaces of 2D materials, showing via molecular dynamics (MD) simulations, that the water slip length increases threefold on hexagonal boron nitride (hBN) in the presence of certain vacancy defects. To this end, I will discuss the use of DFT calculations to assign quantum-mechanically derived partial charges in defective 2D materials. I will also outline the validation of the assigned charges by comparing the predicted electrostatic potential with the quantum-mechanical potential from DFT calculations. Furthermore, I will show that the presence of surface roughness in hBN, but not that of vacancy defects, can explain the experimentally observed water contact angle and slip length on hBN. This finding can be explained by increased electrostatic interactions between hBN edges and water, which lead to higher work of adhesion and friction coefficient of water, resulting in a lower water contact angle and shorter water slip length compared to pristine hBN. Finally, I will discuss how nanopores in 2D materials functionalize in water, outlining the implications for rates of water and ion/boron transport. I will establish the crucial role played by edge charges in modulating nanopore transport through neutral 2D materials. Overall, the multi-scale simulations presented in this talk will help understand and advance the controlled synthesis of nanoporous 2D materials and their applications in nanofluidics and membrane separations.

Theoretical Investigations of Active Sites on Covalent-Organic-Frameworks with Transition-Metal decorated Linkers for Selective CO₂ Utilization

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Selective adsorption of CO₂ from flue stream and natural gases is critically important due to its rising concentration in the atmosphere and its harmful environmental impact. The major impediment in realizing an efficient carbon capture and sequestration strategy stems from identification of an efficient cost-effective CO₂ adsorbent showing exclusive selectivity and high storage capacity with low heat of adsorption, that ensures high recyclability and good thermal, chemical and water stability of the material along with fast kinetics for predominant physical adsorption-desorption mechanism. In this talk, we outline a computational workflow with semi-empirical GFN2-xTB and dispersion-corrected density functional theory to interrogate the effectiveness of six *in silico* designed covalent organic frameworks (COFs) with different linker-bridge-ligand combinations, featuring imine, ethylene and azo-bridges coordinated to 1,10-phenanthroline ligand moieties. > 350 stable adsorption geometries, corresponding association energies and adsorption selectivity on interaction with CO₂, N₂, CH₄, CO and H₂ are discussed. Our theoretical findings demonstrate that azo-bridged COF model consisting of a tetrakis(4-nitrophenyl)-methane linker, with an additional naphthalene moiety coordinated to the ligand exhibited an excellent adsorption selectivity for CO₂ over N₂ (29), CH₄ (39), H₂ (45) and CO (98) under ambient condition (298 K), with -19 kJ mol⁻¹ binding energy for CO₂ adsorption, complying with the requirement of a balanced adsorption capacity and reasonably low heat of adsorption for practical utility. Additionally, we discuss a systematic study with 64 transition-metal decorated adsorbent-gas adducts with Ni, Pd and Pt that shows Pt-COF invariably binds to CO₂ with more favorable binding energy (-16 kJ mol⁻¹) as compared to other gas molecules. Our study outlines how functional group or ligand modifications could be utilized to construct novel materials that could compete with the working capacity of industrially relevant agents under similar conditions.

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Ion-Specific Effects on Electrochemical Interfaces: Water Restructuring, Dynamics, and Spectral Response under Applied Potentials

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Understanding the structure and dynamics of electrified interfaces is crucial for various physicochemical and biological processes. A detailed molecular-level interpretation of electric field effects on interfacial phenomena and ion-induced water restructuring provides fundamental insights across multiple disciplines.^{1,2} Ions influence water structure and dynamics not only at the interface but also in the bulk. This study investigates ion-specific effects in aqueous electrolytes confined between gold electrodes, with one electrode functionalized by a 4-mercaptobenzonitrile (4-MBN) monolayer. Using molecular dynamics simulations, we examine systems with potassium chloride (KCl) and magnesium chloride (MgCl_2) under applied voltages of -2.0, 0, and 2.0 V, employing the constant charge method.³ We analyze structural and dynamic properties, including electric field projections on nitriles, water rotation, and voltage- and ion-dependent hydrogen bond dynamics. Our findings reveal that water dynamics vary with applied voltage and ion identity. While interfacial water typically exhibits slower dynamics than bulk water, KCl addition reverses this trend. In contrast, MgCl_2 does not follow the same behavior, likely due to its structure-making/-breaking properties, aligning with experimental observations. These insights enhance our understanding of voltage-dependent interfacial and bulk water dynamics, ion-specific restructuring at electrochemical interfaces, and their implications for electrochemical reactions, catalysis, biochemical processes, and solar cell applications. Future work will explore concentration-dependent ion-specific responses in water-electrolyte mixtures.

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Freeze Desalination for Fluoride Removal: Performance and Prospects

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Abstract

Excessive fluoride concentration in groundwater presents a severe public health challenge across several states in India, leading to widespread acute fluorosis. While conventional defluoridation strategies—such as the Nalgonda technique, ion exchange, electrochemical, and membrane processes—are widely documented, their field-level application is frequently constrained by heavy chemical sludge production, high operational costs, and intensive maintenance requirements [1]. To address these limitations, decentralized, point-of-use technologies are increasingly vital for rural and semi-urban Indian communities. This study explores the viability of freeze desalination as an alternative, low-chemical defluoridation technique. Operating on the principle of progressive freeze crystallization, the process exploits the physical exclusion of fluoride ions from the growing ice crystal lattice during phase separation [2].

Computational simulations utilizing molecular dynamics (MD) demonstrate that partial freezing can achieve high fluoride removal efficiencies from contaminated water without the need for chemical additives. The efficacy of this technique depends primarily on two coupled phenomena: the rate of ice crystalline growth and the rate of ion rejection. Both mechanisms are highly sensitive to operating parameters, including the degree of supercooling (ΔT), the concentration and chemical species of ions present in the aqueous phase, and the application of external fields (e.g., electric fields, shear stress, and mechanical vibration). In this study, direct co-existence simulations of a 0.15 M solution were conducted using the Madrid-2019 force field to investigate the transport behavior of Na^+ and F^- ions at the ice-solution interface. The results indicate that ion rejection is most efficient near the equilibrium freezing point and decreases monotonically with increasing ΔT . Conversely, the ice growth rate peaks at $\Delta T=15$ K and is significantly suppressed near the freezing point. Furthermore, the application of an external electric field induced a 38.4% increase in F^- removal, achieving an overall ion rejection efficiency of 95%. By leveraging conventional domestic refrigeration conditions, this physical separation method presents a user-friendly, robust alternative for household water purification as well as a primary treatment stage for industrial wastewater.

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Friction and transport in nanoconfined water and electrolytes

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Abstract

For an accurate modeling of nanofluidic systems one needs to understand friction, transport and conduction properties of water and electrolytes in nano-confinement. For this the separation of interfacial from confinement effects is crucial. For the example of planar slit pores, it is shown how surface slip and surface friction can be separated from hydrodynamic bulk-like friction using force correlations from equilibrium simulations without running into the plateau problem. By splitting conductivities and diffusivities into interfacial and confinement contributions, it is demonstrated that confinement effects set in below a confinement width of 1 to 2 nanometers, in agreement with results for the water dielectric tensor [1] and as expected from the orientational interfacial structure of water obtained from non-linear spectroscopy [2].

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October 4-8, 2026

Phase Separation under Anisotropic Conditions

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Abstract

The interplay between phase separation and external driving fields can introduce directional bias, leading to anisotropic phase separation and novel pattern formation that are absent in conventional quench-induced phase separation. At the continuum level, we employ phase field modeling to investigate phase separation under anisotropic conditions generated by a cooling source moving through a liquid¹. The moving source creates a spatially and temporally varying temperature field, continuously driving different regions of the system into the unstable regime. We systematically examine the influence of the cooling-front velocity, source velocity, and composition on the evolving morphology. Our simulations reveal a rich spectrum of anisotropic structures, including concentric rings, wake-like patterns, elongated domains, and droplet morphologies. The observed pattern transitions arise from the interplay between thermal transport and phase-separation kinetics, demonstrating that the externally imposed anisotropy fundamentally alters the coarsening process².

To complement the continuum description, we perform molecular dynamics simulations of a confined two-phase fluid subjected to anisotropic thermal conditions, where the confining walls are maintained at different temperatures. These simulations will provide molecular-level insight into how thermal gradients, confinement, and interfacial interactions influence phase separation and domain evolution, thereby bridging continuum and microscopic descriptions of anisotropic phase separation.

Our combined continuum and molecular approaches provide new insights into nonequilibrium phase separation under directional thermal driving and suggest strategies for controlling microstructure through localized moving heat or cooling sources. The findings are relevant to a broad range of applications including directional solidification, laser-assisted processing, additive manufacturing, and microstructure engineering.

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Crossing Barriers: Stochastic Dynamics of Polymer Translocation

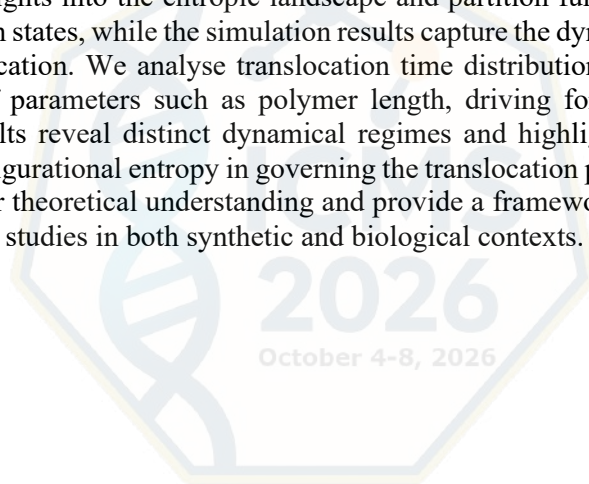
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Abstract

Polymer translocation through narrow pores is a fundamental process with broad relevance, ranging from biological phenomena such as DNA transport through nuclear pores to the development of nanopore-based sequencing technologies. In this work, we investigate the stochastic dynamics of polymer translocation using a combination of exact enumeration techniques and coarse-grained molecular dynamics simulations. The exact enumeration provides detailed insights into the entropic landscape and partition functions associated with different translocation states, while the simulation results capture the dynamic aspects of driven and unbiased translocation. We analyse translocation time distributions, scaling behaviours, and the influence of parameters such as polymer length, driving force, and pore-polymer interaction. Our results reveal distinct dynamical regimes and highlight the critical role of fluctuations and configurational entropy in governing the translocation process. These findings contribute to a deeper theoretical understanding and provide a framework for interpreting and guiding experimental studies in both synthetic and biological contexts.



DNA packing in viral capsids

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Abstract

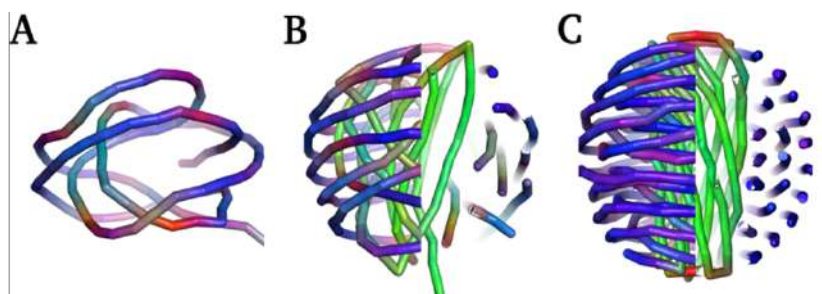
Assembly of viral capsids containing genetic material, is a key process in viral reproduction cycle. The bacteriophages and double stranded DNA viruses assemble their capsids prior to genome packaging and actively push DNA inside by ATP-driven packaging motors. The genome is typically densely packed in the capsid and understanding its spatial configuration presents a challenging problem, which is not completely understood despite its obvious importance.

To elucidate the mechanism of DNA packing, we first explored a simple model of elastic filament confined to a sphere with three competing interactions^[1]. The simple phenomenological theory supported by extensive parallel tempering MD simulations of the wormlike chain (WLC) model show that the optimal ground state packing is not an inverse spool configuration as previously assumed; it is a more complex structure where the filament is compartmentalized into multiple domains, resembling nested tori or topological links. While this suggests that DNA will also form multidomain structures in a viral capsid, it is important to realize that DNA cannot be completely described by the linear elastic model. Under sufficient local torsion, the base pairs of the double helix can locally melt creating regions with large flexibility that can easily form kinks. We incorporated this effect into a meltable WLC model and explored nonequilibrium process of pushing such kinkable chains into a capsid by molecular motors^[2]. It turns out that the kink formation crucially affects the structure: for sufficiently slow packing process we observe a coexistence of outer spool domain and a twisted nematic core – in a perfect agreement with available cryo-EM experimental observations. Our findings suggest that the nonlinear elasticity of biological molecules plays an important role in their spatial structuring in confined biological systems.

October 4-8, 2026

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Spool-nematic packing of kinkable wormlike chain from nonequilibrium MD simulations [2].

Hydration-mediated transport in neutral poly(ethylene oxide) solutions by tuning polymer density heterogeneity

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Abstract

Aqueous solvation shells often govern intermolecular interactions in polymeric and biological systems, yet their role as a control parameter for molecular transport remains largely unresolved. Here, we demonstrate that the addition of ionic salt can regulate molecular diffusion, not primarily through direct electrostatic interactions with probe molecules, but by restructuring the hydration environment surrounding neutral polymers.

Using a combination of fluorescence correlation spectroscopy and molecular dynamics simulations, we show that molecular transport in aqueous poly(ethylene oxide) solutions can be systematically modulated by salt concentration. The transport enhancement is most pronounced near the polymer overlap regime, where small changes in polymer organization produce substantial changes in the heterogeneous local-density landscape. Spatial analysis of the polymer environment reveals that salt redistributes polymer-rich and polymer-lean regions, increasing the availability of low-density pathways through which weakly interacting molecular probes can diffuse more rapidly. Simulations further indicate that ion–polymer proximity modifies polymer hydration and chain conformation, providing a microscopic origin for this density redistribution.

These results suggest a broader physical picture in which hydration-mediated reorganization of polymer density provides a route for controlling molecular transport in neutral crowded media. Rather than ionic strength itself being the fundamental control variable, we propose that changes in the local hydration environment connect molecular-scale ion–water–polymer interactions to mesoscale structural heterogeneity and ultimately to probe diffusion. This framework may provide a useful basis for understanding and designing transport in synthetic polymer solutions and more complex hydrated soft materials, including biologically crowded environments.

Graph neural network-based structural classification of glass-forming liquids

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Abstract

When a liquid is cooled below its melting temperature, it enters a supercooled state while retaining its disordered amorphous structure. As the temperature continues to decrease toward the glass transition temperature, the structural relaxation time experiences a rapid increase, eventually leading to solidification. This phenomenon is commonly referred to as the glass transition. Theoretical and computational elucidation aimed at unraveling the characteristics that govern the slow dynamics in glass-forming liquids, particularly within structures closely similar to those of normal liquids, has presented a formidable problem.

Machine learning (ML) methodologies have been applied for data obtained from molecular dynamics (MD) simulations to explore multifaceted origins of the slow dynamics from the atomistic level. These investigations have effectively opened new perspectives for comprehending the characteristics between liquids and glasses, spanning the prediction of their properties to the elucidation of structural and dynamical changes by varying temperatures. The seamless integration of ML and MD represents a transformative approach, which yields insights into the behaviors inherent to various glass-forming liquids.

Building on recent advances in ML, particularly Graph Neural Networks (GNNs), our study automatically extracts features, unveiling fundamental mechanisms driving structural changes at varying temperatures (Fig. 1). We employ the self-attention mechanism to generate attention coefficients that quantify the importance of connections between graph nodes, providing insights into the rationale behind GNN predictions. By exploring structural changes with decreasing temperature through the GNN+self-attention using physically defined structural descriptors, including the bond-orientational order parameter, Voronoi cell volume, and coordination number, we identify strong correlations between high attention coefficients and more disordered structures as a key indicator of variations in glass-forming liquids.¹

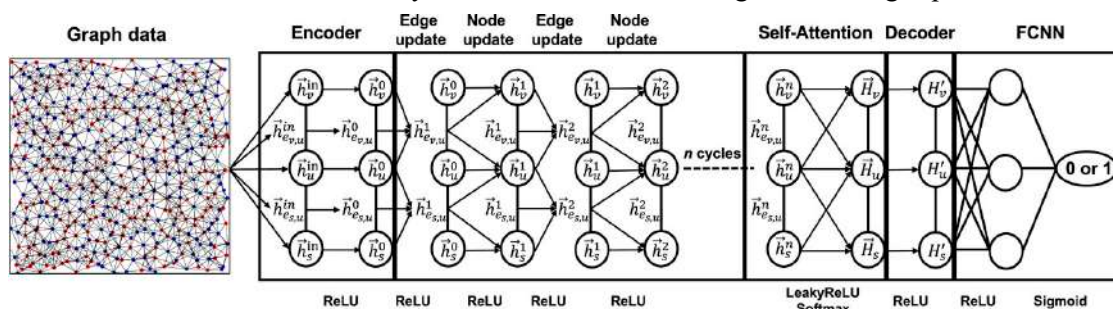


Fig. 1. Schematic picture of the GNN architecture conducted in this study.

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Feedback-controlled relaxation pathways of responsive colloids

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Abstract

Stimuli-responsive colloidal microgels are soft functional materials whose particle sizes dynamically adapt to external fields, local density, and crowding. Such internal responsiveness underlies applications ranging from catalysis to drug delivery, where particle functionality is closely linked to compressibility, permeability, and deformation. While the equilibrium behaviour of responsive colloids has been extensively studied, much less is known about their nonequilibrium relaxation pathways. In particular, the coupling between translational motion and internal size relaxation can generate feedback-controlled dynamics, temporal retardation, and memory effects.

We investigate the nonequilibrium relaxation dynamics of responsive colloidal suspensions using stochastic many-body Brownian dynamics simulations together with coarse-grained theoretical descriptions. Two driving protocols are considered: instantaneous pressure jumps implemented through a Berendsen barostat and continuous compression or expansion using movable confining walls. These protocols enable us to examine how external driving and particle-size responsiveness jointly determine the route to equilibrium.

We find that the relaxation pathways are strongly controlled by the response parameter, $\alpha = D_o/D_T$, which quantifies the ratio of size relaxation to translational diffusion. Depending on α and the driving protocol, the system exhibits asymmetric compression and expansion pathways, transient over- and undershooting of the mean particle size, and counterintuitive cases where slower internal relaxation under confinement leads to faster overall equilibration. We further establish the equilibrium equation of state as a thermodynamic reference for interpreting these nonequilibrium pathways.

Our results demonstrate how internal feedback mechanisms can be used to control relaxation pathways in adaptive colloidal materials, providing a general framework for understanding pathway selection in soft matter far from equilibrium.

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Theoretical Insights into CO₂ Capture and Utilization

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Abstract

The increasing concentration of CO₂ in the atmosphere presents a critical challenge, contributing to climate change and global warming. Carbon Capture and Utilization (CCU) has emerged as a promising approach to reduce atmospheric CO₂ levels while producing valuable products. In our research, the capture and separation of CO₂ from flue gases using metal-organic frameworks (MOFs) have been extensively studied through Grand Canonical Monte Carlo Simulation (GCMC), Molecular Dynamics Simulation, and Density Functional Theory (DFT). We aim to develop high-performance adsorbents for experimental processes such as pressure swing adsorption (PSA) and temperature swing adsorption (TSA).

In addition to CO₂ capture, utilization through electrochemical reduction (CRR) represents a promising pathway for CO₂ recycling and energy regeneration. Our research focuses on developing advanced electrocatalysts with enhanced product selectivity and efficient conversion of CO₂ into valuable C²⁺ products. A major challenge in this process is reducing the barrier for carbon-carbon (C-C) coupling reactions, a critical step for producing multi-carbon products. We employed DFT modelling to gain a molecular-level understanding of the electronic properties of electrocatalysts and their interactions with reaction intermediates. We designed single and dual transition metal-doped two-dimensional (2D) materials as potential catalysts. The results reveal that the oxidation states of transition metals, mainly the d-orbital occupancy, play a pivotal role in modulating the electronic properties of the catalysts. This modulation significantly affects their reactivity, reaction pathways, and product selectivity. By fine-tuning the electronic and structural properties of these materials, our findings provide valuable insights into the design of high-performance electrocatalysts for CRR.

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Data-Driven Material Design: Accelerating Ion Transport Optimization in Solid and Liquid Electrolytes

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Next-generation high-energy-density batteries require electrolyte that simultaneously maximize ion transport and stabilize reactive interfaces. However, traditional development relies heavily on empirical trial-and-error or computationally expensive calculations. This talk presents a machine learning (ML) framework that accelerates design by identifying the underlying structural, chemical, and physical descriptors governing ion dynamics across both solid and liquid phases.

In the solid state, we deploy active-learning interatomic potentials and regression models to isolate the critical features driving lattice and interfacial transport. By evaluating polycrystalline garnet-type and NASICON-structured solid electrolytes, we establish design principles to minimize macroscopic resistance through the optimization of local atomic environments, grain-boundary configurations, and dopant chemistries. We extend this descriptor-centric philosophy to liquid electrolyte design for metal anodes. By introducing "interaction motif" descriptors, we quantify complex ion-solvent interactions spanning from electrostatic to dispersion regimes. These descriptors provide a rational pathway for high-performance liquid formulations. Collectively, this work highlights how physics-informed machine learning shifts the battery materials paradigm from brute-force screening to target-driven synthesis across diverse material phases.

AI-aided accelerated inverse materials design

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Abstract

Mapping desired properties to material structures represents the final frontier of advanced materials design for emerging technologies. Traditionally, materials discovery has relied on trial-and-error experimentation — a process that is slow and costly, consuming significant resources with no guarantee of success. While machine learning-accelerated property prediction has helped narrow the experimental search space, recent advances in generative AI have opened entirely new possibilities: the ability to directly design materials possessing a precisely specified set of properties for a target application.

Earlier generative approaches — Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs) — carry well-known limitations such as mode collapse and posterior collapse and generate a disproportionately large fraction of low-symmetry crystal structures. Diffusion-based models have emerged as a compelling alternative, overcoming these shortcomings and yielding significantly higher-quality crystal structures.

In the backdrop of many sophisticated diffusion models in the literature, I will present the we developed built around a minimalist design philosophy. DiffCrysGen — a powerful, lightweight model — achieves generation throughputs up to two orders of magnitude faster than the leading baseline models. Building on this foundation, DiffCrysGen is adapted to conditional materials generation using classifier free guidance. Accelerated generation throughput, robust materials quality and diversity, and excellent conformation to design targets make both models valuable tools for high-throughput inverse materials design. I will illustrate their capabilities through concrete examples drawn from the design of advanced functional materials.

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Machine learning accelerated screening of positive electrodes for calcium batteries

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Abstract

Calcium batteries (CBs) are a promising beyond-lithium-ion technology, offering the appeal of Ca's natural abundance, standard reduction potential similar to lithium, and high volumetric energy density as a metallic negative electrode. However, practical realization of CBs remains limited by the scarcity of positive electrode (cathode) materials that support reversible Ca^{2+} (de)intercalation under typical electrochemical conditions. To address this challenge, we screen the materials project (MP) database for novel host structures that can intercalate Ca using geometry- and chemistry-based design principles, with acceleration provided by foundational machine learned interatomic potentials (MLIPs). Specifically, we employ the Voronoi polyhedral volume as a descriptor of site compatibility for hosting Ca in potential frameworks, and down-select candidate structures progressively through diverse criteria, including charge neutrality, absence of non-Ca mobile cations, thermodynamic (meta)stability, average voltage, and Ca migration barriers (E_m). Overall, from an initial pool of 52,945 MP structures, our high-throughput workflow identifies 37 promising Ca cathode candidates across 25 distinct compositions, several of which exhibit favorable combinations of thermodynamic (meta)stability, voltage, and Ca^{2+} mobility, marking them as strong candidates for experimental synthesis and electrochemical characterization. Further, we validate a subset of Ca E_m predictions made by MLIPs with density functional theory based calculations as well, highlighting the robustness of our screening approach. Our work establishes geometry-based descriptors and machine learning based workflows as transferable methods for high-throughput screening, enabling the rational discovery of novel materials for various applications.

Zooming inside a Crowded Cell: Lessons from Multiple Resolution Simulations

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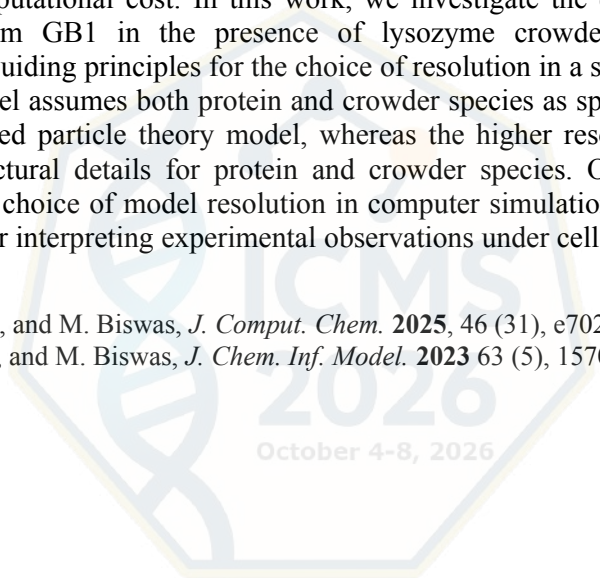
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Abstract

Biochemical reactions occur in a heterogeneous and crowded environment. From a simulation perspective, investigation of crowding effects demands careful consideration of various factors like resolution of the model and interactions, representation of solvent degrees of freedom and computational cost. In this work, we investigate the dimerization of well-studied model system GB1 in the presence of lysozyme crowders at two structural resolutions, seeking guiding principles for the choice of resolution in a simulation model. The lower resolution model assumes both protein and crowder species as spherical beads, similar to the analytical scaled particle theory model, whereas the higher resolution model retains residue specific structural details for protein and crowder species. Our results indicate a nontrivial role of the choice of model resolution in computer simulation studies and provide invaluable insights for interpreting experimental observations under cell-like conditions.^{[1][2]}

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PRIME: A Prediction and Recommendation System for Imputation of Missing Entries in Material Property Matrix

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Gas adsorption isotherms are fundamental to assessing the performance of nanoporous materials in separation applications. Yet, experimental and computational constraints often yield sparse and unevenly distributed data, particularly under technologically relevant conditions such as elevated pressures, higher temperatures, and multicomponent mixtures. This lack of comprehensive datasets hinders the development of robust structure property relationships and limits the efficiency of high-throughput screening strategies.

To address this challenge, we introduce PRIME (Prediction and Recommendation system for Imputation of Missing Entries), a data-driven framework based on the **Generalized Low Rank Model (GLRM)**. By decomposing the sparse material property matrix into low-dimensional latent factors, PRIME uncovers hidden correlations among adsorbates, thermodynamic states, and material chemistries. This enables the imputation of unmeasured adsorption properties from readily available benchmarks, such as nitrogen isotherms at 77 K, with improved accuracy and consistency.

The proposed framework not only enriches incomplete datasets but also functions as a scalable recommendation system to guide material discovery. By reducing dependence on costly or infeasible measurements, PRIME offers a pathway toward accelerating the identification of promising candidates for gas separation applications.

Keywords: Recommendation system, isotherm prediction, metal-organic framework, molecular simulation, machine learning

Figure:

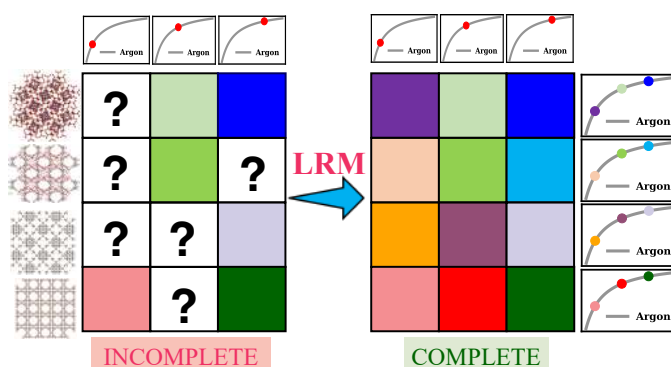


Figure : A schematic illustration of imputing missing entries in the material property matrix by leveraging the known values. Each row corresponds to a distinct material, and each column represents a specific property

Modelling the aggregation of alpha synuclein in presence of neutral crowders

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Abstract

Crowders are indispensable part in cellular environment that effects the formation of Liquid-liquid phase separation (LLPS) in intrinsically disordered proteins (IDPs). Different volumes and sizes of crowders are known to influence the kinetics and structural transformation of the aggregation. However, the specific ways in which crowders modify and manipulate subtle molecular forces are still debated and not well understood. We propose a coarse grain model that elucidates how the same volume percentage of differently sized neutral crowders affects the aggregation pattern of alpha-synuclein. When the size of the crowder is smaller than the protein's radius of gyration (R_g), viscosity effect are found to dominate at higher volume fractions. In contrast, volume-exclusion effect becomes more significant when intermediate-sized crowders are present. Larger crowders can trap protein oligomers within their voids, thereby inhibiting further growth. At higher volume percentage they can also impede the overall aggregation rate while limiting aggregate size. With this study, we were able to show how the kinetics at intermediate volume percentage (10-15 %) of the crowder is different from other volume percentages, especially when the crowder size is comparable to the protein size, which may be the reason for obtaining the LLPS state around this volume percentage experimentally. This highlights the impact of the optimal crowder volume percentage on attaining the LLPS state.

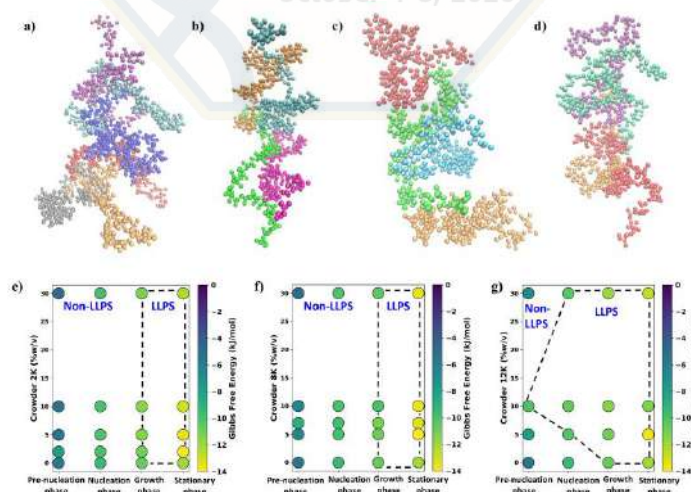


Figure 1. a), b), c), d) Snapshot of the pattern of β -contacts between NAC and the N-terminal region of proteins in the largest aggregate in presence of crowder. Gibbs free energy of transfer computed during the monomer

exchange at different phases of aggregation of alpha-synuclein chains in the presence of **e)** crowder 2K, **f)** crowder 8K, and **g)** crowder 12K.



Calculation of 1 M-Mesh Fine 3D Free Energy Map for Small Molecules in Inhomogeneous Solid Media

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Abstract

A new efficient calculation method has been developed for free energy of transfer of small molecules from vacuum into inhomogeneous media in their low-concentration limit. The method enables us to draw fine three dimensional (3D) free energy maps consisting of one million meshes. The following three techniques were used to enhance calculation efficiency. (1) A new importance sampling method was applied to the free energy calculation according to Widom equation [1]. (2) The method samples thousands of test molecules simultaneously, each of which follows single-particle canonical distribution independently. (3) The test molecules in the media were sampled at high temperatures approximately to accelerate the sampling while the media were at the ambient temperature. Computational cost of the method is much lower than that of the conventional test particle insertion (TPI) method [1] based on inefficient random samplings. This new method can efficiently calculate position-dependent free energy which plays a central role in dynamic Monte Carlo calculations as reported in our previous papers [2-4]. The fine free energy map also presents abundant information about microscopic absorption and diffusion mechanisms of solute molecules.

The method was applied to water molecules in polylactic acid (PLA) and polypropylene (PP). The calculated 3D free energy maps are presented in Fig. 1. Spatially averaged free energy over entire MD cells was in excellent agreement with that obtained by TPI method for both polymers. They also showed a good correspondence to the experimental water absorption rate. These results validate the present method. Analysis showed that water molecules were located in small gaps in the high-density PLA and were stabilized by strong hydrogen bonds with ester polymer chains. In contrast, water molecules were weakly absorbed to PP due to weak van der Waals interactions with its hydrophobic groups, and were distributed in the broad gaps in the low-density PP.

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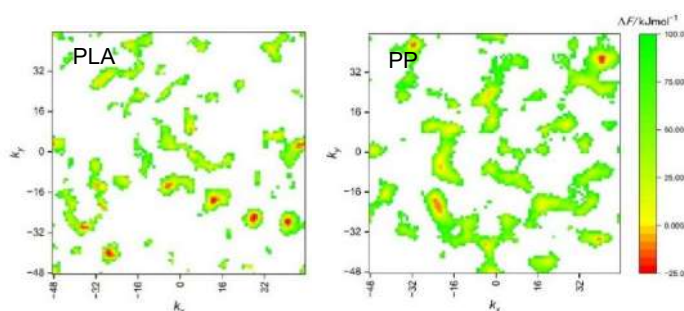


Fig. 1 Cross sections of calculated 3D free energy map of water in its low-concentration limit in PLA and PP. Spatial resolution is 0.05 nm and side lengths of the box are 5 nm.

Insights into ion transport in electrolytes and developing a hybrid Green-Kubo method

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Abstract

Understanding ion transport in electrolyte materials requires resolving the coupled effects of molecular structure, transport, relaxation phenomena, and ion correlations across multiple length and time scales. In this work, molecular dynamics simulations are employed to investigate ion transport behavior in liquid and polymer electrolytes relevant to advanced energy storage systems. For EC-LiTFSI electrolytes spanning a wide concentration range, analysis of ion diffusivity, viscosity, ion-pair relaxation, and ionic conductivity reveals distinct transport regimes. At low salt concentration, ion motion is dominated by vehicular transport, while increasing concentration promotes ion association and collective structural relaxation, leading to structural diffusion. The competition between these mechanisms produces a characteristic nonmonotonic conductivity trend and a unified concentration-dependent description of ionic conductivity over several orders of magnitude in salt concentration via $\sigma \sim c^\alpha e^{-c/c_0}$. In parallel, an efficient hybrid Green-Kubo (hGK) framework is developed for calculating viscosity by combining direct integration of short-time stress correlations with analytical treatment of long-time relaxation dynamics. The approach reproduces benchmark viscosities with dramatically reduced computational cost and remains reliable for concentrated liquid electrolytes and polymer electrolyte systems where conventional Green-Kubo methods fail to converge. These results establish quantitative links between stress relaxation, viscosity, ion-pair dynamics, and ionic conductivity, providing a robust computational framework for the design of next-generation electrolyte materials.

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Predicting long-timescale kinetics from short MD simulations

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Abstract

The dynamics of proteins, including folding and unfolding as well as ligand binding and unbinding, proceed through a number of intermediate states. To elucidate such dynamics based on molecular dynamics (MD) simulations, the Markov state model (MSM)^[1] has been widely utilized. This method enables the description of long-timescale dynamics based on transitions between distinct stable structures. A practical limitation of the MSM method is the need to introduce a coarse-grained timescale, namely, a lag time, in computing transition probabilities. It is known that the resulting kinetic properties can be sensitive to the choice of the lag time.

To overcome this limitation, we propose the integral-equation formalism of population dynamics (IEPDYN) to describe the population dynamics of distinct states ($j = 1, 2, \dots$)^[2]. The phase-space probability density associated with a given state obeys the modified Liouville equation that includes influx from and efflux to neighbouring states. From this equation, one can derive the integral equations governing the state populations at time t , $P_j(t)$, and the population flux from state j to state i at time t , $Q_{ij}(t)$ (Fig. 1). The quantities appearing in these equations (e.g., $K_{ijk}(t)$) are associated with the state-to-state transitions in the local neighborhood of a given state. Thus, they can be computed using a set of short-timescale MD simulations and the long-timescale dynamics can be predicted by solving the set of the integral equations. In addition, thanks to a continuous-time description in the IEPDYN method, kinetic quantities obtained from IEPDYN are free from lag-time dependence.

Fig. 1 (lower panel) illustrates the unbinding kinetics of 18-crown-6-ether (crown ether)/K⁺ in water analyzed with the IEPDYN and brute-force MD simulations. It is found that the IEPDYN method accurately predicts the residence time correlation function (TCF), which is defined as the conditional probability that the pair remains in the bound state at time t , given that it was initially in bound state. The required timescale of each MD trajectory in the IEPDYN method is approximately two orders of magnitude shorter than that of the brute-force MD approach, demonstrating the effectiveness of the IEPDYN method.

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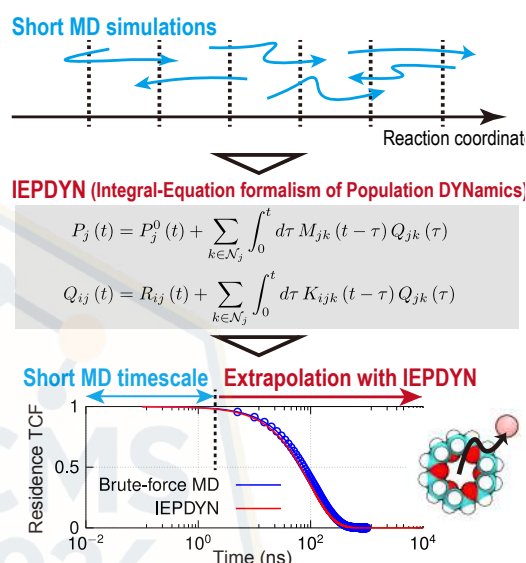


Fig. 1: Prediction of the residence time-correlation function (TCF) associated with the state change based on the short-timescale MD and IEPDYN^[2].

Extracting Reliable Potential of Mean Force for Biomolecules from Molecular Simulations

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Abstract

The Free Energy Landscape (FEL) of biomolecules determines the thermal populations of their conformational states. Further transitions between these states are governed by free energy profiles, termed potentials of mean force (PMFs), drawn along reaction coordinates which connect them. PMFs thus provide insights into thermodynamics, kinetics, and pathways for a wide range of biomolecular processes such as protein activation, enzymatic catalysis, and protein-protein/drug binding. Typically, PMFs for various processes can be constructed from biased molecular dynamics (MD) simulations such as umbrella sampling (US) or metadynamics. However, fundamental unresolved issues including the quality of sampling statistics and reaction coordinates in these simulations limit their abilities to provide reliable PMFs. I will showcase a new software called AutoSIM which uses new foundational insights into the aforementioned issues^{[1][2]} to automate the construction of high quality PMFs directly from biomolecular structures using short MD and US simulations.^[3]

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A Theoretical Framework for Quantifying Frequency-Dependent Signal Transfer in Biomolecules

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Abstract

Cells and organisms respond to external and internal signals through proteins composed of spatially separated sensor and effector modules. The mechanisms by which biological information is transmitted at the molecular level and the timescales of signal propagation, however, remain poorly understood. We use fundamental statistical-mechanics concepts to derive transmit functions^[1] that describe how a local time-dependent perturbation, which can be a deformation or a force, propagates in a viscoelastic medium such as a protein. Transmit functions are defined by equilibrium fluctuations from simulations or experimental observations. Applied to molecular dynamics simulation trajectories of a bacterial histidine kinase protein extensively studied in experiments, our framework reveals that splay deformation of its coiled-coil motif is the biologically relevant signal transmission mode. For the GPCR β_2 -adrenergic receptor — a transmembrane protein involved in the G-protein signaling pathway—our framework enables the quantitative evaluation of signal propagation among the different structural domains, which serve as potential key allosteric hotspots during receptor activation.

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Somananda Sanyal, Wiley

Invited talk

7 October 2026

Parallel Session VI · Hall C

Industry / Special Session

Abstract pending

The abstract for this scheduled talk will be inserted after the submission has been confirmed.



Ritwik Kavathekar, Biovia, Dassault Systemes

Invited talk

7 October 2026

Parallel Session VI · Hall C

Industry / Special Session

Abstract pending

The abstract for this scheduled talk will be inserted after the submission has been confirmed.



Ashutosh, Micropoint Computers Pvt. Ltd.

Invited talk

7 October 2026

Parallel Session VI · Hall C

Industry / Special Session

Abstract pending

The abstract for this scheduled talk will be inserted after the submission has been confirmed.



National Program on Technology Enhanced Learning (NPTEL)

Invited talk

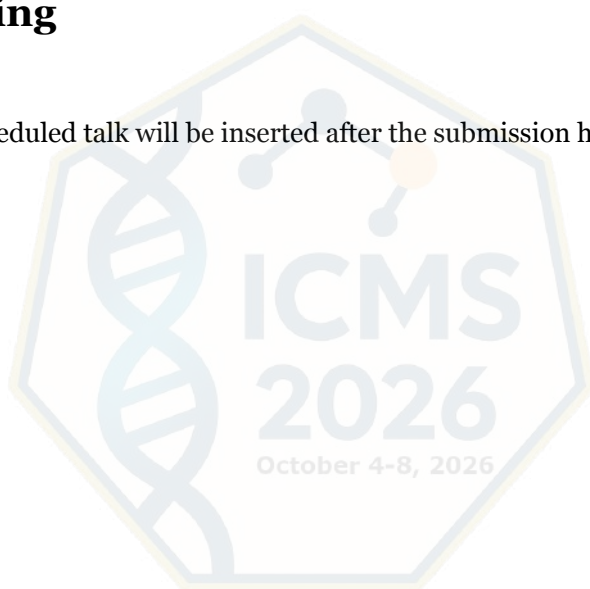
7 October 2026

Parallel Session VI · Hall C

Industry / Special Session

Abstract pending

The abstract for this scheduled talk will be inserted after the submission has been confirmed.



Rational Drug design strategies for IDPs using molecular simulations and machine learning approaches

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Abstract

Highly labile intrinsically disordered proteins (IDPs) are not directly amenable to conventional drug-designing strategies that hinge upon the knowledge of a reference 3-dimensional structure. Physics and machine learning based computational tools, particularly those that incorporate the available experimental information, can be effectively used to generate high-resolution ensemble structures of IDPs and rationally design small molecule inhibitors for these ensemble conformations. I will discuss our recent biomolecular simulations and machine learning based work on small molecule binding properties of A β 42 and α -synuclein, proteins involved in the neurodegenerative proteinopathies, namely, Alzheimer's and Parkinson's diseases, respectively. Our all-atom resolution binding geometries data with accurate conformational ensembles of IDPs in complex with small molecules and peptides provides critical insight towards the rational design of inhibitors for IDP in dilute and condensate phase. We believe that the ML-based pipeline developed by us is general in nature and can be used to cluster and visualize IDP ensembles across systems with varying degrees of structural heterogeneity and assist in detailed structural, thermodynamic, and kinetic analyses of IDP conformations in APO and bound states with small molecules and other partners biomolecules.

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Role of Highly Conserved Central Histidine in the Transport Mechanism of Formate/Nitrite Transporters

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Abstract

Channels and transporters are integral membrane proteins that transport solutes across the cell membranes. Many of them are selective for specific solutes. The family of Formate/Nitrite transporters (FNTs) is selective for monovalent anions [1]. The main metabolites of bacterial respiration during anaerobic mixed-acid fermentation are formate, nitrite and hydrogen sulphide. These anions become cytotoxic when accumulated in cytoplasm. Individual FNT members are involved in selectively transporting these anions. Three-dimensional structures of different FNT members indicate that they share an aquaporin-like hour-glass helical fold. Since FNTs are found only in bacteria, archaea, fungi and protists and not in mammals, they are considered as potential drug targets for many diseases caused by bacteria and fungi.

We performed equilibrium molecular dynamics (MD) simulations and umbrella sampling on FNT members belonging to three representative FNT subfamilies including an uncharacterized subgroup from *Escherichia coli* [2]. The centrally conserved His residue was considered both in protonated and neutral form. We evaluated potential of mean force (PMF) profiles of different solutes using umbrella sampling approach. Our simulation studies strongly suggest that the uncharacterized FNT homolog from *E.coli* is not likely to transport monovalent anions [3]. Its physiological function is perhaps to transport neutral solutes or even cations.

Although the central His is 99% conserved, in the FNT homolog in the amoebiasis-causing *Entamoeba histolytica* (EhFNT), the central His is naturally substituted by Asn. This system is naturally suited to investigate whether central His is protonated or not. Equilibrium MD, umbrella sampling and in silico mutations were carried out on series of FNT systems including EhFNT and FNT homolog from *Vibrio cholerae* (VcFNT). Our studies show that both formate anion and formic acid substrates can be transported through wild-type EhFNT. When Asn is substituted by neutral His, there is a huge energy barrier for the formate anion to be transported. This barrier is significantly reduced when His is protonated. We will discuss the implications of these results in the context of transport mechanism of FNTs.

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From Evolution to Molecular Simulations: Decoding and Engineering Thermostability in an Ancient Protein Fold

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Abstract

The double-psi β -barrel (DPBB) fold [1], one of the most ancient protein architectures capable of forming from minimal amino acid repertoires [2], exhibits remarkable thermostability in modern hyperthermophilic enzymes. Understanding how this primordial fold achieves extreme thermostability in modern hyperthermophilic organisms requires integrating evolutionary, structural, and biophysical perspectives. We present a comprehensive computational framework combining evolutionary mining, structural modeling, multiscale molecular dynamics simulations (18 microseconds across 300–373 K), energetic profiling, and rational redesign to investigate *Thermococcus* AMP phosphorylase thermostability. Analyzing three phylogenetically diverse homologs (*T. kodakarensis*, *T. gammatolerans*, *T. chitonophagus*), we reveal critical stability determinants: restricted conformational dynamics, enriched non-covalent interactions (hydrogen bonds, salt bridges), preserved secondary structure content, and optimized molecular compactness under thermal stress. Free energy landscape analysis demonstrates *T. kodakarensis* occupies deep energy minima with limited conformational fluctuations, contrasting with less stable homologs. Comparative mutational profiling identified destabilizing hotspots, enabling systematic redesign yielding optimized designs with enhanced stability, preserved catalytic function, and strengthened interdomain communication. Stabilizing mutations demonstrated transferability across evolutionary relatives, validating the framework's predictive power. This integration of evolutionary signals, structural dynamics, and energetics provides generalizable design principles for engineering robust biocatalysts, bridging ancient fold simplicity with modern enzyme optimization strategies [3].

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Molecular Modelling of Aptasensor–NCD Biomarker Interactions: Binding Mechanisms and Detection Insights

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Abstract

Human serum albumin (HSA) is a vital biomarker for Non-Communicable Diseases (NCDs). An aptasensor employs a fluorescent dye-conjugated aptamer (short ssDNA) as a probe to detect albumin in a sample. At the beginning, the aptamers are quenched by the adsorption on graphene in a solution. Albumins in a sample then bind to aptamers causing the desorption of aptamer from graphene. This allows the recovery of fluorescent intensity which can be then interpreted into the concentration of albumin in a sample. Recently, the albumin-selective aptamer was discovered by our colleagues where such aptamer was effectively used as a probe. Recently, nano-sized graphene or graphene quantum dot (GQD) has been discovered. It offers superior biocompatibility and lower cytotoxicity which is promising for medical use. Thus, in this work, Molecular Dynamics (MD) simulations were employed to evaluate the feasibility and atomic-level mechanism of a GQD-based aptasensor. The structural and functional properties of albumins were firstly studied and followed by the molecular exploration on how GQD-based aptasensor recognises and detects albumin in a sample. These insights provide a theoretical foundation for optimizing high-sensitivity biosensors with potential diagnostic applications in both human and veterinary medicine.

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Calculation of optimal membrane shape and its application in biology

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Abstract

A biological membrane always tends to optimize its shape by minimizing its free energy. There are several techniques to calculate the optimal shape of a membrane, such as, elastic theory of membrane, Monte Carlo simulation etc. Using elastic theory of membrane, we calculate the optimal shape of a membrane deformed by transmembrane protein transporters during the transport of molecules (such as nutrients, toxins, drugs) across the cell membrane. We use our calculations to explain the role of membrane mechanical properties on the transport process^[1]. Further, we use similar technique to calculate the membrane constriction during membrane scission, and explain the role of membrane tension in the scission process. We also use Monte Carlo simulation to generate optimal membrane shape by discretizing the membrane surface. We find that our model nicely captures the properties of cell migration on flat substrate^[2,5], coiling of cellular protrusions around fibers^[3], as well as cellular migration on curved surfaces^[4].

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Interactions with membrane proteins enable the translocation of surfactant micelles across the bacterial outer membrane

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Abstract:

Recent studies report the abundance of integral membrane proteins in the outer membrane of Gram-negative bacteria [1], challenging the conventional lipid-centric models of membrane organization. This revised understanding of the architecture of the bacterial membrane necessitates a re-examination of how antimicrobial molecules interact with them and eventually permeate this complex biological barrier. Surfactants are one of the most widely used class of antimicrobials in daily life, whose interactions with membranes are complicated by their tendency to aggregate as micelles [2,3]. Using multiscale molecular dynamics simulations, we observe a preferential affinity for micelles to bind to channel proteins in the outer membrane, over lipids. Micelles are observed to bind to the extracellular loops of the channel protein OmpF to result in obstructed channelling of other small molecules. Interestingly, surfactants eventually break free from micelles in this bound state to move further into the channel, suggesting a mechanism through which surfactants permeate through porins despite initially assembling into micelles substantially larger than the pore diameter. We further examined the energetics of complete translocation of a surfactant through the channel by estimating the free energy associated with the process. Using the finite temperature string method, the free energy barrier observed for crossing the constriction region of the channel is examined in a multidimensional collective variable space. These calculations confirm significant affinity for surfactants to enter the channel, while crossing of the constriction region requires conformational acrobatics in the form of folding and flipping leading to a barrier crossing event. Using the above approach, our study provides new insights on how aggregation and structural properties of surfactants lead to differences in mechanism for them to translocate complex membrane barriers.

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Molecular Mechanism of Ice-inhibition by MOF Nanoparticles: Insights from Molecular Simulations

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Abstract

Heterogeneous ice nucleation and ice recrystallization are central challenges in cryopreservation, where uncontrolled ice growth can induce cell damage [1]. Several bio-inspired and synthetic cryoprotective agents, including antifreeze proteins (AFPs) [2], metal–organic frameworks (MOFs)[3], poly(vinyl alcohol) (PVA), graphene oxide (GO)[4], and have demonstrated ice recrystallization inhibition. However, unlike AFPs and polymeric inhibitors, the underlying molecular mechanism of ice inhibition by MOF nanoparticles remains poorly understood because their ice-binding behavior is governed by a complex interplay of surface chemistry, pore environments, hydrogen bonding, interfacial water structure, and nanoparticle size [3,5].

Herein, we present our recent computational investigations into the molecular origins of MOF-mediated ice inhibition using large-scale molecular simulations combined with data-driven analyses. We show that Zr-based MOF nanoparticles, particularly UiO-66 derivatives, organize interfacial water into persistent clusters that anchor to the advancing ice front through extensive hydrogen-bond networks. [3]. These interactions perturb the local ice interface, producing curvature consistent with a Gibbs–Thomson-type growth-arrest mechanism. The nanoparticles exhibit strong adsorption at the ice surface, giving rise to a thermal-hysteresis-like response and suppressing the local melting temperature by approximately 10–12 K [3]. Structural and energetic analyses further reveal the distinct roles of MOF–water interactions and the surrounding hydrogen-bond network in governing ice inhibition. The talk will also compare the mechanisms of ice inhibition by MOFs and antifreeze proteins through heterogeneous nucleation studies using seeding simulations. These calculations reveal fundamentally different free-energy landscapes and interfacial interactions, providing new molecular insights into how synthetic nanoparticles and biological macromolecules suppress ice formation. Finally, the influence of mechanical perturbations on nucleation pathways will be discussed, highlighting the interplay between shear, interfacial ordering, and ice-growth arrest. Together, these findings establish a molecular framework for understanding MOF-mediated ice inhibition and provide design principles for developing next-generation cryoprotective materials with enhanced ice recrystallization inhibition performance.

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Elucidating the Evolving Nature of DNA Graphene Interactions Using Polarizable Simulations

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Graphene has garnered remarkable attention in recent years as an attractive nanopore membrane for rapid and accurate sequencing of DNA. The inherent characteristics of graphene offer exquisite experimental control over pore dimensions, encompassing both width (pore diameter) and height. Despite these promising prospects, the practical deployment of pristine graphene nanopores for DNA sequencing has encountered a formidable challenge in the form of pore clogging, primarily attributed to hydrophobic interactions. However, a comprehensive understanding of the atomistic origins underpinning this clogging phenomenon and the nuanced impact of individual nucleobase identities on clogging dynamics remains an underexplored domain. Elucidating the atomistic intricacies governing pore clogging is pivotal to devising strategies for its mitigation and advancing our comprehension of graphene nanopore behaviour.

Utilizing an innovative methodology, we harness Drude polarizable simulations to systematically dissect the nucleobase-dependent mechanisms that play a pivotal role in nanopore clogging. The polarizable simulations were used to establish the interactions between nucleobases and graphene surface, studying the self-assembly of these nucleobases on the graphene surface before studying the nanopore dynamics. We unveil nucleobase-specific interactions that illuminate the multifaceted roles played by both hydrophobic and electrostatic forces in driving nanopore clogging events. Notably, the Drude simulations also unveil the bias-dependent translocation dynamics and its pivotal role in alleviating pore clogging—a facet that remains significantly underestimated in conventional additive simulations. Our findings underscore the indispensability of incorporating polarizability to faithfully capture the intricate dynamics governing graphene nanopore translocation phenomena, thus deepening our insights into this crucial field.¹⁻⁵



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Polarizable Model of Graphitic Materials for Accurate In-Silico Nanoscopy

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Abstract:

Graphitic materials are of immense scientific and technological importance owing to their tunable electrical conductivity, adjustable band gap, excellent thermal properties, and high strength-to-weight ratio. These materials have widespread applications in batteries and fuel cells as electrode materials, refractory components, and lubricants, as well as in nuclear reactors, aerospace technologies, water purification, steel manufacturing, and biosensing. In this work, we present a realistic, all-atom polarizable model of graphite that features flexible dummy electrons to explicitly capture the electron cloud polarization in graphitic structures. Following the IFF (Interface Force Field) validation protocol, the model predicts the density, lattice parameters, surface energy, hydration energy, water contact angle, and elastic constants within approximately 1%, 1%, 5%, 5%, 5%, and 15% of experimental values, respectively. Furthermore, it accurately reproduces experimental and density functional theory (DFT) data for the binding energies and interaction profiles of cations (Na^+ , Li^+), anions (F^- , Cl^- , Br^-), and neutral molecules, including water and amino acids. The model also demonstrates a substantial improvement in predicting water–graphite interfacial friction, a key parameter governing nanoscale hydrodynamics. An accurate molecular-level description of these interfaces is essential for the rational design of graphitic materials with tailored interfacial and transport properties.

Investigating Defect-Mediated Gas Transport and Separation in CNTs Using Atomistic Simulations

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Abstract

Defect-free carbon nanotubes (CNTs) are known to exhibit exceptional mass transport, with remarkably high gas permeation rates owing to atomically smooth carbon lattices that lead to a low Maxwell reflection coefficient.¹⁻⁴ However, in practice, the synthesis of defect-free CNTs is extremely challenging, often leading to the formation of various structural defects that can significantly influence transport properties.⁵⁻⁶ The influence of defects on the Maxwell reflection coefficient and, consequently, on gas transport and separation performance remains unknown. In this work, we investigate the role of defects in CNTs on gas transport and H₂/CH₄ separation performance by employing equilibrium molecular dynamics (EMD) simulations. We examine the most commonly reported single vacancies and Stone-Wales defects in CNTs to systematically evaluate their impact on gas diffusion and separation performance. Our simulations show that these defects significantly attenuate gas transport, resulting in diffusion coefficients up to two orders of magnitude lower than those of the corresponding defect-free CNTs. Further, a key outcome of this investigation is the development of an effective Maxwell reflection coefficient to describe defect-induced transport. Our results indicate that the effective Maxwell reflection coefficient for defected CNTs can be expressed through a simple linear relationship with the intrinsic reflection behavior of pristine CNTs, providing a simple model to predict defect-modified transport at any given defect concentration. Furthermore, defects affect the transport of CH₄ more than that of H₂, enhancing H₂/CH₄ separation performance in defected CNTs. Overall, this study provides molecular-level insights into defect-mediated gas transport in carbon nanotubes and establishes a predictive framework linking structural defects to gas transport behaviour, offering guidance for the rational design of CNT-based separation membranes.

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Deciphering Gas Hydrate Nucleation Through Machine Learning-Based Polymorph Classification and Molecular Simulations

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Abstract

Understanding the kinetics and mechanisms of nucleation during crystallisation is crucial for technological advancement. Molecular simulations play an important and complementary role to experiments by providing detailed molecular insights into nucleation processes. To analyse nucleation trajectories, crystalline order parameters are used to classify molecules into different phases, but designing these parameters is often complex and time-consuming. In this work, we focus on obtaining order parameters capable of identifying and classifying natural gas hydrates into different polymorphs. Starting from a set of generic order parameters [1], we systematically determine a minimal subset that can differentiate between water molecules across various polymorphs of gas hydrates using machine learning. Specifically, we train the XGBoost [2] machine learning model to classify water molecules as belonging to liquid, ice-Ih, ice-Ic, sI, sII, or sH hydrates. This model is then applied to analyse methane hydrate nucleation near a planar gas-liquid water interface, with the nucleation rate calculated via the mean first passage time (MFPT) formalism [3]. Our model's performance is compared with previously developed order parameters from the literature [4], showing that a minimal set of generic order parameters can accurately classify different crystal polymorphs, eliminating the need to develop specialised order parameters for each material under investigation. Furthermore, the developed machine learning model is also used to obtain the composition of the formed cluster. Results show that the critical nucleus formed has a disordered mixture of hydrate phases, with no dominant crystalline structure, indicating an amorphous nature.

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Understanding Light Oil – Rock Interactions using Molecular Dynamics Simulations

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Abstract

In enhanced oil recovery, the extraction efficiency of injecting fluids (IFLs) heavily relies on the adsorption behavior of crude oil on rock surfaces. Therefore, a detailed understanding of oil–rock interactions is crucial when designing efficient IFLs for crude oil extraction. In this work, we performed molecular dynamics simulations to probe the structure and energetics of light oil (dodecane) near carbonate (calcite), clay-type (mica), and sandstone (silica) reservoir surfaces. We found that light oil exhibits a layered distribution near the surfaces, with a strong bound layer on calcite that is absent on the other surfaces. The light oil molecules preferentially adsorb parallel to the surface, with epitaxial adsorption over the calcium ions of the calcite surface, whereas structured adsorption is observed over the oxygen atoms and silicate chains of the mica and silica surfaces, respectively. The adsorption strength, determining the presence or absence of the bound layer, is primarily governed by the strong net-interaction energy between the rock surface and the oil, which is dominated by van der Waals interactions. In contrast, the distinctive adsorption pattern observed on each rock surface is attributed to local, atomic-level electrostatic interactions. Based on our comprehensive analysis, we provide recommendations for IFL design.

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A multiscale computational approach to identify novel viral epitopes by targeting pMHC-TCR complexation

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T-cell immunity is a crucial defense against viral infections in vertebrates. Upon viral entry, innate immune cells process viral proteins and present them via Major Histocompatibility Complex (MHC) molecules. T-cell receptors (TCRs) recognize these MHC-bound viral peptides (pMHC), initiating a T-cell-mediated immune response. Despite its significance, the mechanism by which pMHC-TCR binding triggers T-cell activation remains unclear, limiting current epitope prediction methods to MHC-peptide binding and not TCR engagement which is essential for immune activation. In this study, we employed an integrative computational approach combining Bioinformatics, Molecular Dynamics (MD) simulations and Machine Learning (ML) to introduce an additional layer for viral epitope screening based on their ability to activate TCRs, while also elucidating the TCR conformational changes underlying immune activation. We performed large-scale all-atom and coarse-grained MD simulations on MHC-peptide-TCR complexes embedded in dendritic and T-cell membranes, with known experimental immunogenicity data. One hundred fifty such systems were simulated for 1 μ s each to capture the conformational and dynamical changes that underlie T-cell activation. Simulation-derived structural and dynamical features were used to develop a multivariate time-series binary classification model, revealing key determinants of T-cell activation, achieving ~76% accuracy in immunogenicity prediction. We also identified the bending of the TCR transmembrane region and the buried surface area between pMHC and TCR as key factors influencing T-cell immune response activation, among others. Model robustness was further validated across epitopes from multiple viruses, with an accuracy of 73%. Our approach unravels the mechanism of T-cell-mediated immune response and helps ML-guided screening of viral epitopes for vaccine development.

From Molecules to Mixtures to Multilayer Devices: A Hierarchical Machine Learning Framework for Materials Discovery

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Abstract

Modern materials are rarely used in isolation — individual materials are typically combined into multicomponent mixtures, or formulations, and many devices are built as a stack of multiple such formulated layers, each layer drawing on similar underlying material building blocks. Predicting end-use device performance therefore requires models that scale coherently across three levels of organization: the material, the formulation, and the layered device. We present a hierarchical machine learning framework that constructs this chain directly, using physics-informed descriptors at each level to preserve mechanistic signal while enabling rapid, data-driven prediction.

At the material level, structural fingerprints are combined with physics-based descriptors from quantum mechanics and molecular dynamics to build predictive models linking material structure to properties. These material-level features are then embedded into composition-aware, permutation-invariant formulation models. Finally, formulation-level features from each layer are aggregated and concatenated across the full device stack to predict whole-device performance.

By linking material, formulation, and device-level models within a single featurization and learning framework, this approach turns traditionally sequential, trial-and-error formulation and device engineering into a unified, predictive design workflow — reducing experimental burden while retaining physical interpretability at every scale. In this talk, I will illustrate this framework with two case studies: a shampoo formulation for the mixture-level model, and a multilayer OLED stack for the device-level model, where predicted device performance reproduces experimental trends in external quantum efficiency and emission color.

Machine Learning of Polymer Phase Transitions

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Abstract

Machine learning (ML) and artificial intelligence (AI) have remarkable abilities to classify, recognize, and characterize complex patterns and trends in large data sets. Here, we adopt a subclass of ML methods, viz., deep learning, and develop a general-purpose AI for analyzing molecular dynamics (MD) trajectories and predicting phases and phase transitions in polymers. An unsupervised deep neural network (DNN) is used within this framework to map a MD trajectory undergoing thermophysical treatment such as cooling, heating, drying, and compression to a lower dimension. A supervised DNN is subsequently developed based on the lower dimensional data to characterize the phases and phase transitions. As a proof of concept, we employ this framework to study the coil to globule phase transition of a model polymer system. We conduct coarse-grained MD simulations to collect MD trajectories of a single polymer chain over a wide range of temperatures and use this framework to predict polymer phases. The framework accurately predicts the critical temperatures for the coil to globule transition for a wide range of polymer sizes. This method is generic and can be extended to capture various other phase transitions and dynamical crossovers in polymers and other soft materials.

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Swarm Intelligence Guided Global Minima Search on Complex Potential Energy Surfaces

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Abstract

One of the current-day challenges in theoretical chemistry is the optimization of complex chemical systems with a large number of degrees of freedom.^[1] The potential energy surfaces associated with the non-covalent interactions involving nanostructures and atomic or molecular clusters are often rugged, with a large number of local minima hindering the tracking down of the global minima. Global optimization techniques are indispensable for attaining the global minimum configurations of such complex systems.^{[1],[2]} In this talk, I shall describe how particle swarm optimization (PSO), one of the swarm intelligence techniques falling under the general ambit of artificial intelligence, can be leveraged for the global optimization of complex chemical systems.^{[3],[4]} Within the domain of structure prediction, I shall highlight a hierarchy of PSO implementations based on the complexity in modeling. I shall further describe some of our recently explored optimal theoretical design strategies for investigating the binding of atomic and molecular clusters with nanostructures by amalgamating various empirical models of intermolecular interactions with PSO.^{[5]-[9]} Such strategies were applied to model a range of applications of carbon nanostructures, including mono- and multi-layered graphene and graphynes, in gas storage and separation, water desalination, *etc.* The combination of PSO with empirical potentials provides an optimal balance between computational efficiency and accuracy in determining the structures and energetics of adsorbed and intercalated clusters of atoms and molecules.

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An Artificial Intelligence enabled virtual screening of natural product space to Identify Hit Molecules against Breast Cancer Subtypes

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Abstract

Many natural sources (plants/microbes/marine products) remain unexplored and they can be a good source of databases from which compound libraries can be generated. With virtual screening, the quality of the hits improves with more number of compounds screened. As we are in AI era, human-AI partnership provides the best of both worlds creating more value than either can do it alone. Artificial intelligence (AI)-driven approaches provides very economical yet highly reliable access to carry out virtual screening of ultra large compound libraries (Chemical spaces/billions of compounds). Even though the current breast cancer therapies respond to conventional chemotherapies, they are associated with some limitations such as resistance, pressured index therapy, non-selectivity, and severe adverse effects. Exploring chemical space/natural sources and artificial intelligence will be helpful in the drug discovery process to identify new drug candidate for the treatment of breast cancer to overcome these limitations. In this study, structure based and ligand based virtual screening was carried out on natural product space using open AI (deep learning tools) ^[1]. After virtual screening, filtering of the active compounds was done based on docking score and Rescoring and clustering of active compounds in two stages. After analyzing the docking data, it was observed that natural products such as flavonoids and some non-flavonoids showed better docking scores against estrogen receptors than progesterone receptor, PARP and HER2. So, the flavonoids (phytoestrogens) were taken for molecular dynamics simulation studies. Molecular dynamics studies indicated the stability of the top scored compounds and the required mode of binding is significant. MM-GBSA implies good affinity of these compounds with ER subtypes. Pharmacokinetic evaluation using Qikprop yielded key findings such as good human oral absorption, poor Blood Brain Barrier permeability and less toxicity. The in silico investigation highlights the prenylated phytoestrogens as anti-breast cancer agents through their selective

ER- β modulatory activity. Based on their favorable pharmacokinetic profiles, high affinity, and specific binding mode, these compounds can be considered as new candidates with potent anti-breast cancer activity. On the other hand, three dihydrochalcones, namely NHDC, SIE and TLN were taken for extensive analysis to reveal their ER α activity. The in vitro cell line study shows good cytotoxicity effect against MDA MB231 and MCF 7 cell lines. This study integrates the AI and natural space to identify unexplored phyto estrogens as hit molecules that can be further optimized into lead moieties.

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Back - extraction of Competing Metal Ions from Oil Phase to Aqueous Phase Using Molecular Dynamics Simulations

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The extraction and back – extraction processes are the important steps for recovery of any metal ions from the waste stream. Both are governed by the interface, and the associated interfacial properties. The ion transfer across the liquid–liquid interface is a complex chemical process, and understanding its fundamentals is crucial for efficient and cost-effective mass transfer. Earlier we performed the back – extraction studies with uranyl ions and found TBP/dodecane system exhibited higher recovery of uranyl ions. Here, the ion-transfer process becomes even more complex for radionuclide metal ions, particularly in the presence of other competing metal ions in the medium, which is the case in PUREX process. Metal ion extraction is fundamentally a complexation process, while back-extraction involves decomplexation, both of which are governed by the interface.¹ These complexation and decomplexation events occur via the water-finger mechanism, where the water finger serves as a pathway for metal ion transfer.² Further, these phenomena can also be expressed through structural effect.³⁻⁴ Now, the co-stripping or co-back extraction of the metal ions has been carried out where the influence of other metal ions may alter the previous trend of recovery of uranyl ions during back- extraction process. Therefore, the molecular dynamics (MD) simulations have been performed with GROMACS simulation package to model the more complex back-extraction process which includes three metal ions such as, uranyl, plutonium and zirconium. These three metal ions are the major components of spent nuclear fuel. The organic phase used three types of ligands such as, including TBP, TiAP and TODGA in dodecane. The stripping agent is pure water. The simulation boxes filled with all the aqueous and organic molecules to allow the complex formation followed by decomplexation. The efficiency of back-extraction of uranyl ion into pure water from TiAP/dodecane phase has been enhanced in presence of other ions. The distribution coefficients (K_D) of uranyl ion, Plutonium ion and zirconium ion have been evaluated for these back – extraction and was found similar to the experimental studies.

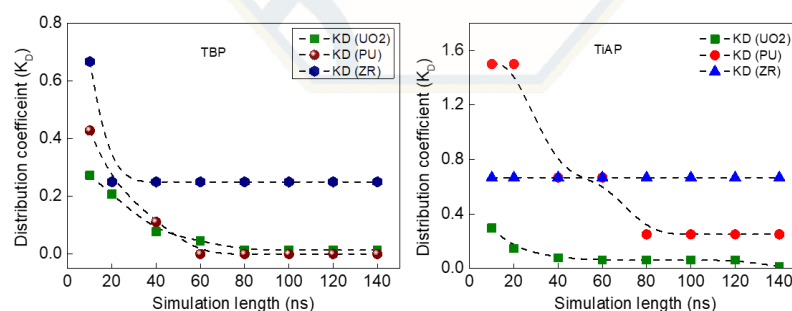


Figure 1. Distribution coefficient of UO_2^{2+} , Pu and Zr during back – extraction

The above figure demonstrated that the uranyl ions exhibited lowest K_D among the others. Lower K_D values result in higher recovery. The recovery of Pu is comparatively higher in TBP/dodecane system.

Acknowledgements: Computer division for providing Anupam super computation facility. Shri. H. R. Pimparkar, CE, NRB, Shri K. T. Shenoy, Director ChEG, BARC, Shri T. Morzaria (GM-PDD), NRB, Smt. B. M. Biswas (AGM-RP), NRB for continuous support and encouragement.

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Comparative Study of ν -shape and S-shape Fibril Elongation: Mechanistic Insights into Templated Assembly and Interfacial Frustration

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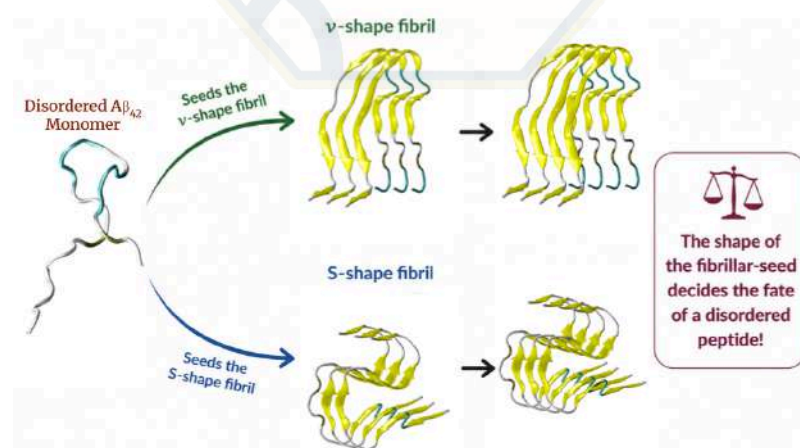
Abstract

Amyloid fibril elongation is a key process in Alzheimer's disease, proceeding through a complex “dock-and-lock” mechanism in which monomers bind, search for the correct registry, and integrate into the growing fibril. Although amyloid- β ($A\beta_{42}$) fibrils exhibit pronounced structural polymorphism, how fibril architecture influences elongation kinetics remains unclear.

In this study, we present a comparative computational study of ν -shaped (PDB: 8EZD) and S-shaped (PDB: 7Q4M) $A\beta_{42}$ trimeric fibrils using the PathGennie¹ path-generation framework and adaptive molecular dynamics simulations. A hierarchical hydrogen-bond-based state model and deep-learning-assisted (VAMPnet) kinetic analysis were employed to characterize the conformational and kinetic landscapes of monomer incorporation.

We found that a common kinetic checkpoint in both polymorphs: productive elongation requires initial anchoring of the β_2 strand. Beyond this point, however, the growth mechanisms diverge substantially. The S-shaped polymorph follows a relatively direct dock-and-lock pathway, rapidly progressing toward the native fibrillar state. In contrast, the ν -shaped polymorph explores a rugged free-energy landscape populated by frustrated and misregistered intermediates that capture nearly 53% of the kinetic flux, significantly delaying elongation.

These findings demonstrate that fibril polymorphism directly controls the extent of kinetic frustration during assembly. By linking fibril architecture to elongation pathways, this work provides molecular insight into the distinct propagation behaviors and potentially the differential toxicities of $A\beta_{42}$ polymorphs.



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Molecular models for Gram-positive bacterial strains: Assessing membrane properties and small molecule interactions

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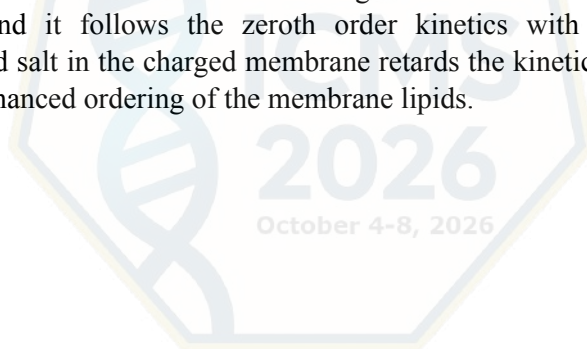
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Abstract

We present a comparative study of the inner membrane of three Gram-positive bacterial strains, namely *Staphylococcus aureus*, *Staphylococcus epidermidis* and *Nesterenkonia lacusekhoensis*. We have developed coarse grained (CG) Martini-3 membrane models which reproduce structural and Mechanical properties. Using the CG models we evaluated the insertion free energies for cecropin-melittin-15 (CM15). Our simulations revealed two distinct membrane binding modes of CM15 with the CG membrane models. We also explored the kinetics of partitioning of thymol molecule with atomistic membrane of *Nesterenkonia* at different charge states of membrane and salt environment. Following the first order kinetics, the thymol molecules spontaneously enter into the charge-neutral membrane. While the cloud of counter-ions in the charged membrane case poses an entry barrier for the thymol insertion and it follows the zeroth order kinetics with a time constant of 1.5 microseconds. The added salt in the charged membrane retards the kinetics with change in counter-ion condensation and enhanced ordering of the membrane lipids.



Atomistic Understanding Radiation Impact on the Leaching Behavior of Sodium Borosilicate Glass

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Abstract

Extensive molecular dynamics (MD) simulations were conducted to elucidate the radiation effect on the aqueous corrosion of the sodium borosilicate glass. Cascade evolution profiles for density, BO_4 fraction, and non-bridging oxygen (NBO) content exhibited asymptotic saturation at a deposited energy of $5\text{--}6 \times 10^{19} \text{ keV/cm}^3$. A pivotal structural transition, $\text{BO}_4 \rightarrow \text{BO}_3 + \text{NBO}$, was observed, accompanied by a shift in the role of Na^+ ions from charge compensators to network modifiers. This transition led to broadening of RDF peaks, bond-angle shifts, and depolymerization. Irradiated glass showed higher network disorder with a 4.87% rise in total entropy and $\sim 35\%$ increase in configurational entropy, as evaluated using very efficient and robust two phase thermodynamic (2PT) method. Macroscopic changes included a 2% density rise, 8.66% decrease in Young's modulus, and 5.8% reduction in T_g . Along with mechanical degradation, results revealed 17.7% higher leach rates in irradiated glass. Simulations across 1–70 keV PKA energies showed that structural damage scaled with total deposited energy. Overlapping of structural profiles for PKA energies below 10 keV, suggest that structural recovery is feasible at lower recoil energies. The findings suggest that while NBS glass may undergo moderate structural and chemical degradation, it will retain long-term stability under repository conditions. The present studies may boost the ongoing global research on simplified borosilicate glass for immobilization of nuclear waste.

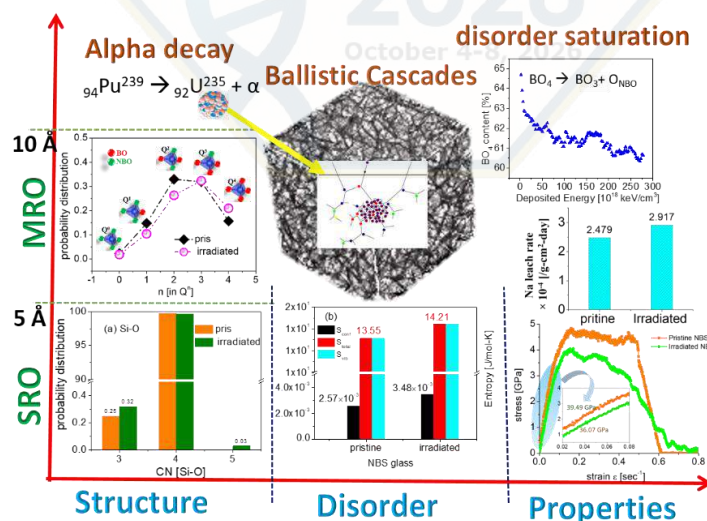


Figure 1. Effect of Radiation cascades on glass disorder and leaching behavior

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Molecular Dynamics and Potential of Mean Force Analysis of PVC–Plasticizer Interactions for the Rational Design of Safer Plasticizers

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Abstract

Atomistic molecular dynamics (MD) simulations combined with potential of mean force (PMF) calculations were performed to investigate the interactions between polyvinyl chloride (PVC) chains containing 6–20 repeating units and a diverse set of plasticizers, with the objective of identifying safer alternatives to the widely used but toxic plasticizer di(2-ethylhexyl)phthalate (DEHP) in blood bags. The investigated plasticizers represent multiple chemical families, including orthophthalates, citrates, adipates, and the terephthalate DEHT. Since both PVC and the plasticizers lack ionizable functional groups, their interactions are predominantly governed by van der Waals and electrostatic forces.

A generalized model correlating PMF profiles with interaction forces was developed and validated across four PVC chain lengths and all 14 investigated plasticizers. The model provides molecular-level insight into how variations in plasticizer structure influence interaction strength and binding affinity toward PVC. Based on the calculated PMF profiles, the plasticizers were ranked according to their binding affinities, identifying TOTM (tris(2-ethylhexyl) trimellitate, TEHTM), BTHC (butyryl trihexyl citrate, Citroflex B-6), ATHC (acetyl trihexyl citrate, Citroflex A-6/CA-6), and DEHT (bis(2-ethylhexyl) terephthalate, DOTP/DEHTP) as the most promising candidates for further evaluation.

The reported results are based on averages from 30 independent simulations for each polymer–plasticizer system, providing a statistically robust comparison across all systems. Beyond identifying promising DEHP alternatives, this work establishes a molecular framework for understanding and predicting PVC–plasticizer compatibility. The proposed methodology facilitates the rational design of polymer–plasticizer systems for applications involving extractables and leachables, supports the development of coarse-grained simulation models, and provides valuable guidance for the design of safer plasticizers for biomedical and advanced materials applications.

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Understanding the Nature of Hydration of Aqueous Alkali Metal Carbonates Employing Molecular Dynamics Simulations

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Abstract

Aqueous alkali metal carbonates (M_2CO_3 , where $M = Li^+$, Na^+ , and K^+) have attracted significant attention due to their critical role in CO_2 capture, energy storage, and various industrial processes. Despite extensive experimental progress in understanding their macroscopic properties, the molecular-level mechanisms governing solvation and ion-association behaviour in these systems with varying concentrations remain largely unexplored. To address this gap, we present a comprehensive molecular dynamics (MD) investigation of aqueous Li_2CO_3 , Na_2CO_3 , and K_2CO_3 using a refined force field model, validated against the experimental solubility limits of the respective salts.^[1] The study highlights how the local environment of carbonate ions (CO_3^{2-}) evolves with solute concentration, highlighting the role of alkali metal cations in promoting the self-aggregation of carbonates. Trajectory analysis predicts that the mobility of all solute and solvent species decreases with concentration, leading to the co-movement of cations and carbonate ions near their solubility limit. Notably, Li^+ exhibits anomalously slow diffusion compared to the larger Na^+ and K^+ ions, owing to its stronger association with carbonate ions, which is consistent with the experimentally observed low solubility of Li_2CO_3 in water. This behaviour is attributed to the size-sensitive “hardness” of cation hydration shells, corroborated in terms of the water residence times in their first hydration shells. Together, these results facilitate a fresh molecular-level understanding of the diverse physical properties of aqueous alkali metal carbonates and have significant implications for the development of CO_2 capture strategies.

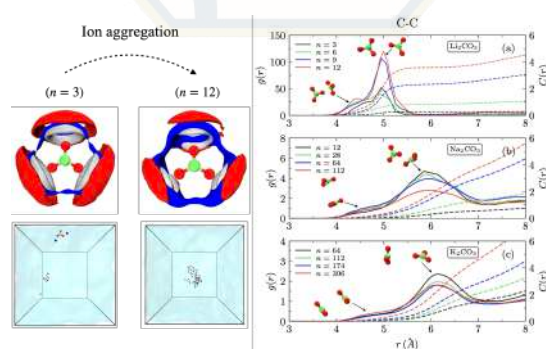


Figure 1 Left: Hydration isosurfaces around CO_3^{2-} at low (dilute) and high (beyond solubility) concentrations with corresponding simulation snapshots showing the transition from dispersed ions to aggregates. Right: Carbonate–carbonate RDFs (solid lines) and coordination numbers, RCNs (dashed lines), for $C \cdots C$ correlations in aqueous Li_2CO_3 , Na_2CO_3 , and K_2CO_3 , quantifying enhanced ion aggregation at higher concentrations.

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Accelerating Self-Assembly through “FAST Water”

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Abstract

Molecular dynamics simulations are a powerful tool for elucidating the molecular mechanisms of supramolecular self-assembly, but the long timescales of aggregation often make all-atom simulations computationally demanding. Here, we evaluate the recently developed TIP3P-FAST^[1] water (or simply, “FAST water”) model as a simple strategy to accelerate self-assembly simulations in aqueous solution. FAST water employs mass repartitioning within a water molecule, increasing molecular mobility without altering the underlying potential energy surface. We investigate representative self-assembling systems with distinct aggregation mechanisms and resultant morphologies^[2]. Simulations of isolated solutes reveal a round 3 fold increase in diffusion coefficients and rotational motion in FAST water compared to conventional TIP3P water, while solvent-accessible surface areas, radial distribution functions, hydrogen-bonding characteristics, and interaction energies remain unchanged. Self-assembly simulations initiated from dispersed monomers show markedly accelerated aggregation kinetics in FAST water, and lower monomer lifetime in case of monomer exchange, while preserving the dissociation kinetics. These results demonstrate that FAST substantially reduces the computational cost of atomistic self-assembly simulations while preserving equilibrium structural and thermodynamic properties, providing a practical route for studying complex supramolecular systems.

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