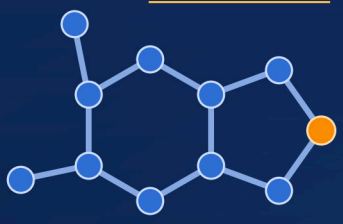
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# Frontiers of Physical Chemistry

*Experiments, Computations and Theory*

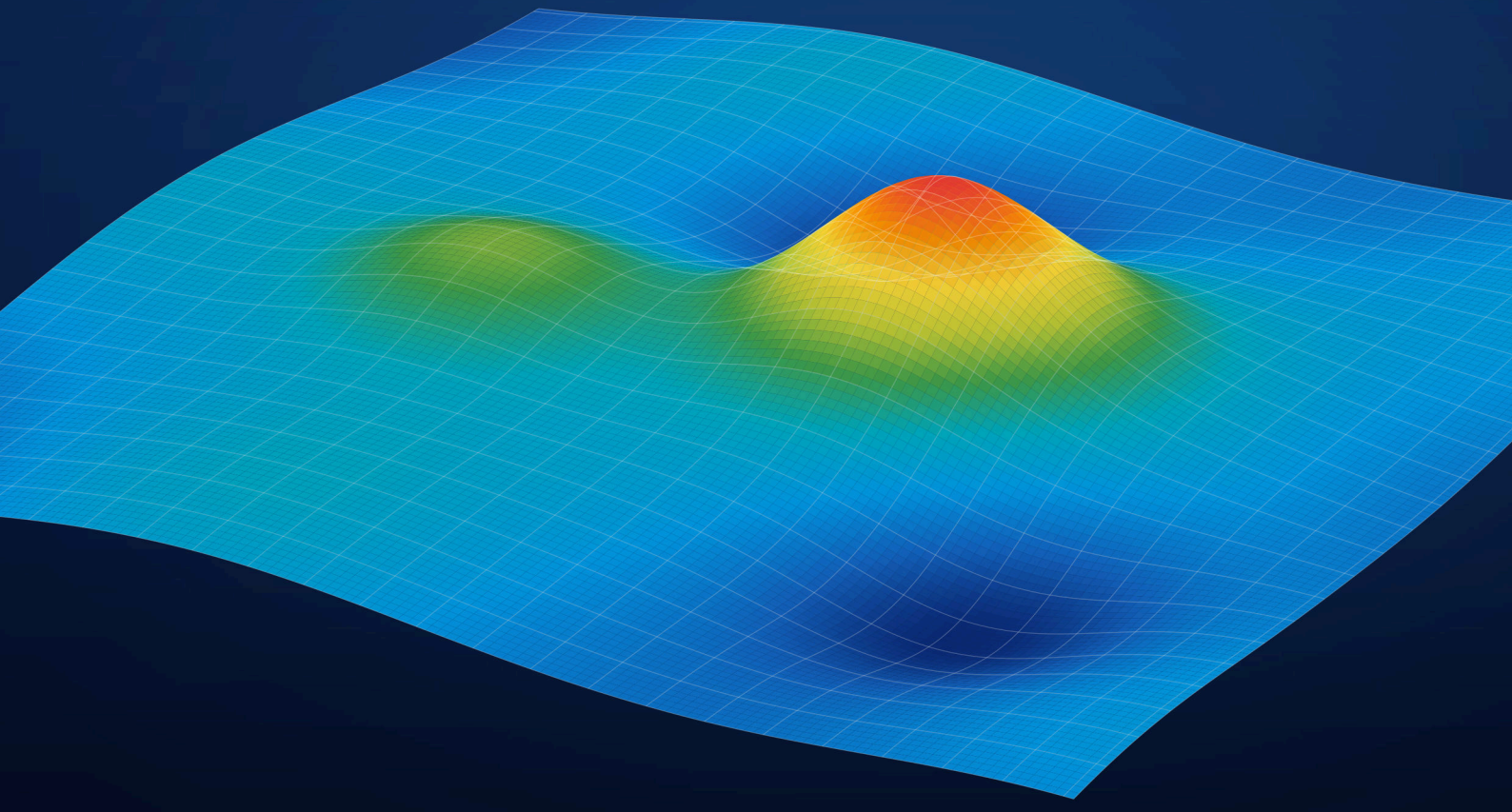
**BOOK OF ABSTRACTS**

WITH THE COMPLETE PROGRAMME



## 28 – 31 October 2026

S. N. Bose National Centre for Basic Sciences, Kolkata



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## JOINTLY ORGANISED BY

S. N. Bose National Centre for Basic Sciences Kolkata

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28 – 31 October 2026 · S. N. Bose National Centre for Basic Sciences, Kolkata

# Welcome from the Conveners

Dear Colleagues and Friends,

It is our great pleasure to welcome you to Frontiers of Physical Chemistry 2026 at the S. N. Bose National Centre for Basic Sciences, Kolkata. Over four days, from 28 to 31 October, the meeting brings together experimentalists, theorists and computational scientists working across the breadth of physical chemistry — ultrafast and nonlinear spectroscopy, chemical reaction dynamics, biophysical chemistry, soft matter and materials, electronic structure and statistical mechanics, and the fast-growing use of artificial intelligence and machine learning in the chemical sciences.

The scientific programme opens each morning with lectures and closes each evening with a special lecture delivered online. It includes the Sadhan Basu and Mihir Chowdhury Oration Lectures, a commemorative session remembering the life and works of Professor B. M. Deb, and 59 invited lectures. True to the tradition of physical chemistry meetings in India, faculty members present posters alongside young researchers: the three poster sessions together carry 26 invited faculty posters and 103 contributed posters. We hope the posters, as much as the lectures, will be where conversations start.

This book collects the full programme, the poster lists and the abstracts, each marked with the same code that appears in the programme. In this soft copy every code and title in the programme tables is a link to its abstract, and every abstract page carries a button that takes you back to the programme.

We are grateful to the members of the National Advisory Committee for their guidance; to the session chairs, speakers and poster presenters; to our sponsors for their generous support; and to the administration of the Centre and the many members of the Local Organizing Committee — faculty, staff and students — whose work has made this meeting possible.

We wish you an engaging and enjoyable conference, and a pleasant stay in Kolkata.

*Ranjit Biswas* *Suman Chakrabarty*

Conveners, FPC 2026 · S. N. Bose National Centre for Basic Sciences, Kolkata

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All entries are clickable


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**How to use this book.** Every code and title in the programme and poster tables is a link to its abstract; each abstract page has a *Back to programme* button. Codes: SBO / MCO — named oration lectures; IL, SL — invited lectures; EL — special evening lecture (online); CL — commemorative lecture; IP — invited faculty poster; P — contributed poster; SP — sponsor talk. Entries without a link had no abstract at the time of compilation.

# Programme at a Glance

Click a session to jump to its detailed listing

| Day 1 | Wednesday, 28 October 2026 |
|---|---|
| 08:00–09:00 | *Registration and distribution of conference kits* |
| 09:00–09:15 | *Inaugural Session* |
| 09:15–10:30 | **Session 1**<br>IL-01–SL-01 |
| 10:30–11:00 | *Tea Break* |
| 11:00–12:45 | **Session 2**<br>IL-04–SL-02 |
| 12:45–14:00 | *Lunch* |
| 14:00–15:15 | **Session 3**<br>IL-08–SL-03 |
| 15:15–15:45 | *Tea Break* |
| 15:45–16:40 | **Session 4**<br>IL-11–SL-04 |
| 16:45–18:15 | **Session 5**<br>Poster Session A |
| 18:15–18:30 | *Break* |
| 18:30–19:30 | **Session 6**<br>Evening Lecture (online): Biman Bagchi |
| 19:30 | *Dinner (SNBNCBS)* |

| Day 2 | Thursday, 29 October 2026 |
|---|---|
| 09:00–10:30 | **Session 7**<br>Sadhan Basu Oration: Amalendu Chandra + 3 talks |
| 10:30–11:00 | *Tea Break* |
| 11:00–12:45 | **Session 8**<br>IL-16–SL-07 |
| 12:45–14:00 | *Lunch* |
| 14:00–15:15 | **Session 9**<br>SL-08–SL-12 |
| 15:15–15:45 | *Tea Break* |
| 15:45–16:45 | **Session 10**<br>IL-19–IL-21 |
| 16:45–18:15 | **Session 11**<br>Poster Session B |
| 18:15–18:30 | *Break* |
| 18:30–19:30 | **Session 12**<br>Evening Lecture (online): Sudipta Maiti |
| 19:30 | *Conference Dinner — Hotel The Sojourn* |

| Day 3 | Friday, 30 October 2026 |
|---|---|
| 09:00–10:30 | **Session 13**<br>Mihir Chowdhury Oration: Tapas Chakraborty + 3 talks |
| 10:30–11:00 | *Tea Break* |
| 11:00–12:45 | **Session 14**<br>IL-25–SL-13 |
| 12:45–14:00 | *Lunch* |
| 14:00–15:25 | **Session 15**<br>IL-29–SL-16 |
| 15:25–15:55 | *Tea Break* |
| 15:55–16:55 | **Session 16**<br>SL-17–SL-20 |
| 16:55–18:25 | **Session 17**<br>Poster Session C |
| 18:25–18:30 | *Break* |
| 18:30–19:30 | **Session 18**<br>Evening Lecture (online): Mark Maroncelli |
| 19:30 | *Dinner (SNBNCBS)* |

| Day 4 | Saturday, 31 October 2026 |
|---|---|
| 09:00–10:30 | **Session 19**<br>IL-31–SL-22 |
| 10:30–11:00 | *Tea Break* |
| 11:00–12:20 | **Session 20**<br>IL-34–SL-24 |
| 12:20–13:20 | **Session 21**<br>B. M. Deb Commemorative Lecture: Swapan K. Ghosh |
| 13:20–13:50 | *Valedictory Session* |
| 13:50–14:50 | *Lunch and departure* |

# Day 1 *Wednesday, 28 October 2026*

| | | |
|---|---|---|
| 08:00 – 09:00 | | *Registration and distribution of conference kits* |
| 09:00 – 09:15 | | **Inaugural Session** |
| **Session 1** | | Chair: Swati De (University of Kalyani) |
| 09:15 – 09:35 | IL-01 | **E. Arunan** (IISc Bengaluru)<br>*Is the distance between two atoms enough to conclude about bonding?* |
| 09:35 – 09:55 | IL-02 | **Sarika Maitra Bhattacharyya** (CSIR-NCL Pune)<br>*Beyond Crystallization Frustration: Structure and Dynamics in Model Glass Former* |
| 09:55 – 10:15 | IL-03 | **Pradipta Bandyopadhyay** (JNU New Delhi)<br>*Generalizing Physics-based Machine Learning for prediction of hydration free energies* |
| 10:15 – 10:30 | SL-01 | **Srestha Basu** (SINP Kolkata)<br>*Engineering Chemical Reactivity and Optical Response through Defect Design in Nanocluster Assemblies* |
| 10:30 – 11:00 | | *Tea Break* |
| **Session 2** | | Chair: Sumana Dutta (IIT Guwahati) |
| 11:00 – 11:20 | IL-04 | **Moloy Sarkar** (NISER Bhubaneswar)<br>*From Surface Chemistry to Excited-State Reactivity: Unraveling Catalysis in Mono- and Bimetallic Nanoclusters* |
| 11:20 – 11:40 | IL-05 | **Durba Roy** (BITS Pilani, Hyderabad)<br>*What Nonequilibrium Work Theorems Tell Us About Carbohydrate Mechanics* |
| 11:40 – 12:00 | IL-06 | **Partha Hazra** (IISER Pune)<br>*TADF-Enabled Triplet Exciton Harvesting in Novel Organic Multifunctional Luminogens* |
| 12:00 – 12:20 | IL-07 | **Ankan Paul** (IACS Kolkata)<br>*Shedding Light on the Mechanism of Highly Selective Toluene Photooxidation under Nano-Confinement* |
| 12:20 – 12:35 | SL-02 | **Saumyak Mukherjee** (IISER Berhampur)<br>*A Bayesian Lens on Molecular Rigidity: Learning Atomic Weights from Ensemble Data* |
| 12:35 – 12:45 | SP-1 | Sponsor Talk — Somananda Sanyal (Wiley-VCH) |
| 12:45 – 14:00 | | *Lunch* |
| **Session 3** | | Chair: Pratim Chattaraj (SNBNCBS Kolkata) |
| 14:00 – 14:20 | IL-08 | **Snehasis Daschakraborty** (IIT Patna)<br>*$CO_2$ Adsorption in Humid COFs: A Transition Matrix Monte Carlo Study* |
| 14:20 – 14:40 | IL-09 | **Biman Jana** (IACS Kolkata)<br>*Learning Transferable Collective Variables For Ligand Binding Transition Through Explainable Machine Learning* |

| | | |
|---|---|---|
| 14:40 – 15:00 | IL-10 | **Debashis Barik** (University of Hyderabad)<br>*Power-law scaling of depth of the potential wells in bistable systems* |
| 15:00 – 15:15 | SL-03 | **Supratik Sen Mojumdar** (IIT Palakkad)<br>*Small-Molecule-Directed Self-Assembly of Amino Acids for Emergent Fluorescence* |
| 15:15 – 15:45 | | *Tea Break* |
| **Session 4** | | Chair: Debashree Ghosh (IACS Kolkata) |
| 15:45 – 16:05 | IL-11 | **Srabani Taraphder** (IIT Kharagpur)<br>*Free Energy and Kinetics of Unbinding of Enzyme Inhibitors* |
| 16:05 – 16:25 | IL-12 | **Debasis Koley** (IISER Kolkata)<br>*In Silico mechanistic rationalization of Copper-complex catalyzed oxidative reactions* |
| 16:25 – 16:40 | SL-04 | **T. Rajagopala Rao** (IIT Patna)<br>*Quantum Nuclear Dynamics: Reactive Scattering and Vibronic Coupling* |
| **Session 5 — Poster Session A** | | Chair: Surajit Maity (IIT Hyderabad) |
| 16:45 – 18:15 | P-A | **Poster Session A** (list of posters, p. 15)<br>Invited faculty posters: IP-01 to IP-07<br>Contributed posters: P-001 to P-033, P-035, P-036 |
| 18:15 – 18:30 | | *Break* |
| **Session 6 — Special Evening Lecture (online)** | | Chair: Anindya Datta (INST Mohali) |
| 18:30 – 19:30 | EL-1 | **Biman Bagchi** (IISc Bengaluru) ONLINE<br>*From Molecular Chirality to Living Helices: Symmetry Breaking, Cooperativity, and Handedness Selection* |
| 19:30 | | *Dinner (SNBNCBS)* |

# Day 2 *Thursday, 29 October 2026*

| Session 7 | | Chair: Anunay Samanta (University of Hyderabad) |
|---|---|---|
| 09:00 – 09:30 | SBO | **SADHAN BASU ORATION LECTURE**<br>**Amalendu Chandra** (IIT Kanpur)<br>*Nonlinear Vibrational Spectroscopic Calculations of the Dynamics of Aqueous Solutions at Charged Interfaces* |
| 09:30 – 09:50 | IL-13 | **Varadharajan Srinivasan** (IISER Bhopal)<br>*An analytical hydrodynamic model for coupled edge plasmons in TMD nanoflakes* |
| 09:50 – 10:10 | IL-14 | **Parbati Biswas** (University of Delhi)<br>*Rheology of Block Copolymeric Ring Polymers in Dilute Solutions* |
| 10:10 – 10:30 | IL-15 | **Vivek Tiwari** (IISc Bengaluru)<br>*What is the electronic character evolution in singlet fission dimers?* |
| 10:30 – 11:00 | | *Tea Break* |
| **Session 8** | | Chair: Rama Kant (University of Delhi) |
| 11:00 – 11:20 | IL-16 | **Aloke Das** (IISER Pune)<br>*β-Turn Peptides: Bridging Molecular Structure and Functional Materials* |
| 11:20 – 11:40 | IL-17 | **Arnab Mukherjee** (IISER Pune)<br>*Memory Effects and Ruggedness as Microscopic Sources of Internal Friction in Chemical and Biophysical Dynamics* |
| 11:40 – 12:00 | IL-18 | **Prasun Kumar Mandal** (IISER Kolkata)<br>*Does Excitation Energy Transfer Happen in Doped Perovskite Nanocrystal?* |
| 12:00 – 12:15 | SL-05 | **Mainak Sadhukhan** (IIT Kanpur)<br>*A systematic Green's function formalism for kinetic energy density* |
| 12:15 – 12:30 | SL-06 | **Anirban Mondal** (IIT Gandhinagar)<br>*From Descriptors to Discovery: A Physics-Informed Inverse Design Framework for Self-Trapped Excitons in Unexplored Halide Perovskites* |
| 12:30 – 12:45 | SL-07 | **Partha Pratim Roy** (IIT Gandhinagar)<br>*Ultrafast Mapping of Nonradiative and Radiative Pathways in Dual-Conformer TADF Emitters* |
| 12:45 – 14:00 | | *Lunch* |
| **Session 9** | | Chair: Sanjay Kumar (IIT Madras) |
| 14:00 – 14:15 | SL-08 | **Arijit Kumar De** (IISER Mohali)<br>*Unveiling Time-Dependent Vibronic Coupling by Third- and Fifth-order Raman Spectroscopy* |
| 14:15 – 14:30 | SL-09 | **Madhurima Jana** (NIT Rourkela)<br>*Hydrophobic Amino Acid Solutions at Work: Do They Reshape Protein Solvation and Thermal Stability?* |
| 14:30 – 14:45 | SL-10 | **Barun Kumar Maity** (SINP Kolkata)<br>*Specific DNA Recognition Induces Folding Transition of the Oncogenic Fusion Protein PAX3FOXO1* |

| | | |
|---|---|---|
| 14:45 – 15:00 | SL-11 | **Debasish Mondal** (IIT Tirupati)<br>*Reset Controlled Non-equilibrium Transition in an Inhomogeneous Brownian Information Engine* |
| 15:00 – 15:15 | SL-12 | **Somrita Ray** (IISER Berhampur)<br>*Stochastic Resetting Prevails Over Sharp Restart for Broad Target Distributions* |
| 15:15 – 15:45 | | *Tea Break* |
| **Session 10** | | Chair: Sabyashachi Mishra (IIT Kharagpur) |
| 15:45 – 16:05 | IL-19 | **Susmita Roy** (IISER Kolkata)<br>*Ions as Molecular Architects Shaping RNA Folding* |
| 16:05 – 16:25 | IL-20 | **Himansu Sekhar Biswal** (NISER Bhubaneswar)<br>*From Conformer Resolution to Bond Scission: An Integrated Approach Using REMPI, RIDIR, and VCD/ECD Spectroscopy* |
| 16:25 – 16:45 | IL-21 | **Sanjoy Bandyopadhyay** (IIT Kharagpur)<br>*Modified Interfacial Environment around Biomolecules in Aqueous Ionic Liquid Mixtures* |
| **Session 11 — Poster Session B** | | Chair: Niladri Patra (IIT (ISM) Dhanbad) |
| 16:45 – 18:15 | P-B | **Poster Session B** (list of posters, p. 18)<br>Invited faculty posters: IP-08 to IP-17, IP-27<br>Contributed posters: P-037 to P-069, P-105, P-106 |
| 18:15 – 18:30 | | *Break* |
| **Session 12 — Special Evening Lecture (online)** | | Chair: Amalendu Chandra (IIT Kanpur) |
| 18:30 – 19:30 | EL-2 | **Sudipta Maiti** (BITS Pilani, Hyderabad) ONLINE<br>*Deep tech in photonics needs talent, ideas, resources, AND deep experience: let's put them together* |
| 19:30 | | *Conference Dinner — Hotel The Sojourn* |

# Day 3 *Friday, 30 October 2026*

| Session 13 | | Chair: Sourav Pal (Ashoka University) |
|---|---|---|
| 09:00 – 09:30 | MCO | **MIHIR CHOWDHURY ORATION LECTURE**<br>**Tapas Chakraborty** (MAKAUT, West Bengal)<br>*Mass Spectrometry in Physical Chemistry Research* |
| 09:30 – 09:50 | IL-22 | **Rajesh Murarka** (IISER Bhopal)<br>*Understanding the coil-globule transition in semi-flexible polymers from an energy landscape perspective* |
| 09:50 – 10:10 | IL-23 | **Ranganathan Subramanian** (IIT Patna)<br>*Atmospheric Oxidation Kinetics of Emerging Halogenated Oxygenated Volatile Organic Compounds (XOVOCs)* |
| 10:10 – 10:30 | IL-24 | **Anirban Misra** (University of North Bengal)<br>*Theoretical Design and Electronic-Structure Engineering of Donor–Acceptor $\pi$-Conjugated Molecular Systems for Tunable Nonlinear Optical Properties* |
| 10:30 – 11:00 | | *Tea Break* |
| **Session 14** | | Chair: V. Subramanian (SRMIST Chennai) |
| 11:00 – 11:20 | IL-25 | **Mousumi Das** (IISER Kolkata)<br>*Role of excited states in optoelectronics: A model exact and DMRG study* |
| 11:20 – 11:40 | IL-26 | **Hemant Kumar Kashyap** (IIT Delhi)<br>*Insights Into Antibacterial Action of Transition Metal Dichalcogenides* |
| 11:40 – 12:00 | IL-27 | **Tushar Debnath** (Shiv Nadar University)<br>*Exciton-Plasmon Coupling in Plasmonic Perovskite Nanocrystals* |
| 12:00 – 12:20 | IL-28 | **Sanjib Senapati** (IIT Madras)<br>*Reinventing the Drug Formulation Technology for Improved Onset of Action and Lower Dose Requirements* |
| 12:20 – 12:35 | SL-13 | **Arnab Halder** (Presidency University, Kolkata)<br>*Role of Photoinduced Processes to Modulate the Optical Properties of Carbon Nanoparticles* |
| 12:35 – 12:45 | SP-2 | Sponsor Talk — Laser Science Services (India) |
| 12:45 – 14:00 | | *Lunch* |
| **Session 15** | | Chair: Sanjib Bagchi (RKM Vivekananda Centenary College, Rahara) |
| 14:00 – 14:20 | IL-29 | **Ayan Datta** (IACS Kolkata)<br>*Buckling and Defects in Two-Dimensional Atomically Thin Monolayers* |
| 14:20 – 14:40 | IL-30 | **Manik Pradhan** (SNBNCBS Kolkata)<br>*Cavity Ring-down Spectroscopy in Gas and Condensed Phases* |
| 14:40 – 14:55 | SL-14 | **Tatini Rakshit** (Shiv Nadar University)<br>*Probing cancer biomarkers using a biophysical approach* |
| 14:55 – 15:10 | SL-15 | **Tapta Kanchan Roy** (University of Delhi)<br>*An Efficient Variational Approach for Thermal Density Matrices with Quantum Anharmonic Effects* |

| | | |
|---|---|---|
| 15:10 – 15:25 | SL-16 | **Atanu Singha Roy** (NIT Meghalaya)<br>*Protein Corona Modulated Doxorubicin Loading and Release from Catechin-Functionalized Ag–Au Alloy Nanoparticles* |
| 15:25 – 15:55 | | *Tea Break* |

**Session 16** — Chair: Avisek Das (IACS Kolkata)

| | | |
|---|---|---|
| 15:55 – 16:10 | SL-17 | **Samiran Sen** (Institut Pasteur, Paris)<br>*Learning what to trust: A Bayesian framework for protein model refinement* |
| 16:10 – 16:25 | SL-18 | **Brindaban Modak** (BARC Mumbai)<br>*Density Functional Theory Study of Single-Atom Catalysts on Porphyrin-like Porous Fullerene for Energy Applications* |
| 16:25 – 16:40 | SL-19 | **Anupam Bera** (University of Hyderabad)<br>*Molecular Structure and Ultrafast Charge-Transfer Dynamics at Functional Material Interfaces: Insights from VSFG and Transient Absorption Spectroscopy* |
| 16:40 – 16:55 | SL-20 | **Suman Das** (GITAM University, Visakhapatnam)<br>*Proteins in Deep Eutectic Solvents: Molecular Insights from Simulations* |

**Session 17 — Poster Session C** — Chair: Debabrata Seth (IIT Patna)

| | | |
|---|---|---|
| 16:55 – 18:25 | P-C | **Poster Session C** (list of posters, p. 21)<br>Invited faculty posters: IP-18 to IP-22, IP-24 to IP-26<br>Contributed posters: P-070, P-072 to P-089, P-091 to P-104 |
| 18:25 – 18:30 | | *Break* |

**Session 18 — Special Evening Lecture (online)** — Chair: Ranjit Biswas (SNBNCBS Kolkata)

| | | |
|---|---|---|
| 18:30 – 19:30 | EL-3 | **Mark Maroncelli** (Penn State University, USA) ONLINE<br>*Adventures of a Lonely Water Molecule as Told by IR, FIR, NMR Spectroscopy and MD Simulation* |
| 19:30 | | *Dinner (SNBNCBS)* |

# Day 4 *Saturday, 31 October 2026*

| Session 19 | | Chair: Ranjan Das (West Bengal State University) |
|---|---|---|
| 09:00 – 09:20 | IL-31 | **Musharaf Ali** (BARC Mumbai)<br>*Thermophysical and dynamical properties of liquid sodium: Insights from MD simulations and DFT-BTE theory* |
| 09:20 – 09:40 | IL-32 | **Sayan Bagchi** (CSIR-NCL Pune)<br>*Water Dynamics in Biomolecular Condensates: Beyond Slow Biomolecular Diffusion* |
| 09:40 – 10:00 | IL-33 | **Milan Hazra** (IIT Jodhpur)<br>*Decoding Molecular Grammar of Heterotypic Biomolecular Condensates: Interplay of Sequence Architecture and RNA-like polyelectrolyte Mediated Competitive Interactions* |
| 10:00 – 10:15 | SL-21 | **Biswajit Guchhait** (Shiv Nadar University)<br>*Domain-Specific Dynamics and Solvent-Controlled Excited-State Proton Transfer in Deep Eutectic Solvents* |
| 10:15 – 10:30 | SL-22 | **Rakesh S. Singh** (IISER Tirupati)<br>*From Interactions to Architecture: Rational Design of Biomolecular Condensate Morphologies* |
| 10:30 – 11:00 | | *Tea Break* |
| **Session 20** | | Chair: Chaitali Mukhopadhyay (University of Calcutta) |
| 11:00 – 11:20 | IL-34 | **Pradipta Purkayastha** (IISER Kolkata)<br>*Epitaxial Assembly of 1D/2D Organic Lateral Heterojunctions for Integrated Photonics* |
| 11:20 – 11:40 | IL-35 | **Rahul Sharma** (St. Xavier's College (Autonomous), Kolkata)<br>*Transient collective motion and density voids in a model drying chemotactic bacterial film* |
| 11:40 – 11:55 | SL-23 | **Satyapriya Bhandari** (Kandi Raj College)<br>*Engineered Nanoarchitectures for Enhanced Energy Transfer and Multifunctional Applications* |
| 11:55 – 12:10 | SL-24 | **Piyush Mishra** (IIT Kharagpur)<br>*Understanding Chemical Mechanisms Through Molecular Spectroscopy* |
| 12:10 – 12:20 | SP-3 | Sponsor Talk |
| **Session 21 — Commemorative Session Remembering the Life and Works of Prof. B. M. Deb**<br>Chair: Pratim Chattaraj (SNBNCBS Kolkata) | | |
| 12:20 – 13:20 | CL | **Swapan K. Ghosh** (UM-DAE Centre for Excellence in Basic Sciences, Mumbai) ONLINE<br>*Commemorative Lecture* |
| 13:20 – 13:50 | | **Valedictory Session** |
| 13:50 – 14:50 | | *Lunch and departure* |

# Poster Session A

Day 1 · Wed, 28 Oct 2026 · 16:45 – 18:15 · Session 5 · Chair: Surajit Maity (IIT Hyderabad)

| No. | Presenter | Title |
|---|---|---|
| **Invited Faculty Posters** | | 7 posters |
| IP-01 | **Bidyut Sarkar**<br>Shiv Nadar University | *Investigation of conformational dynamics and ligand binding mechanism of gene regulatory SAM-II / SAM-V tandem riboswitch* |
| IP-02 | **Niladri Patra**<br>IIT (ISM) Dhanbad | *Mapping Conformational and Kinetic Landscapes of 14-3-3σ/α-Synuclein Assembly via Variational Autoencoders and Markov State Models* |
| IP-03 | **Saumyak Mukherjee**<br>IISER Berhampur<br>abstract with SL-02 | *A Bayesian Lens on Molecular Rigidity: Learning Atomic Weights from Ensemble Data* |
| IP-04 | **Debdas Dhabal**<br>IIT Guwahati | *CMA-ES-based Force Field Parameter Optimization of Diiodomethane for Surface Free Energy Calculations* |
| IP-05 | **Pradip K. Ghorai**<br>IISER Kolkata | *Breaking Azeotropes: The Role of Entrainers in Efficient Separation* |
| IP-06 | **Papri Chakraborty**<br>IIT Kharagpur | *Activation of atomically precise monolayer-protected Pt nanoclusters: Formation of active CO oxidation catalysts* |
| IP-07 | **Utpal Sarkar**<br>Assam University, Silchar | *Machine Learning Approach to Screen Potential Donor and Acceptor Fragments: Insights from Chemical Reactivity* |
| **Contributed Posters** | | 35 posters |
| P-001 | **Hirak Jyoti Baishya**<br>IIT Guwahati | *Targeting Plasmodium Falciparum Purine Nucleoside Phosphorylase (PfPNP) with Unnatural Nucleosides: A Computational Study* |
| P-002 | **Surendra Nath Barman**<br>NIT Meghalaya | *BSA Conjugated Carbon Nanotubes for Release of Potent Antioxidant Curcumin* |
| P-003 | **Keniya Basu**<br>University of Calcutta | *On the origin of the structural isomerism dependent intersystem crossing : role of spin–orbit and nuclear motion assisted spin–orbit coupling* |
| P-004 | **Saswata Basu**<br>IIT Kanpur | *Quantum phase transitions in time-dependent quantum mechanical scattering* |
| P-005 | **Suman Bhowmik**<br>IIT Kanpur | *Decoding Intersystem Crossing: Molecular Design, Vibrational Control and Environmental Modulation* |
| P-006 | **Partha Pratim Borah**<br>IIT Guwahati | *Rethinking Activity Descriptors for Single-Atom Iron Water Oxidation Catalysts* |
| P-007 | **Roohi Choudhury**<br>NIT Meghalaya | *Deciphering bio-nano interfaces of AgNPs and Ag2SNPs with HSA: mechanistic insights into protein-nanoparticle complexation and their effects on antibacterial activity* |
| P-008 | **Subhajit Dan**<br>IIT Kanpur | *Unraveling the Dynamics of Interfacial Water at Electrified Graphene Surfaces through Theoretical Two-Dimensional Vibrational Sum-Frequency Generation Spectroscopic Study* |

| No. | Presenter | Title |
|---|---|---|
| P-009 | **Hrishika Dey**<br>IIT (ISM) Dhanbad | *Targeting Plasmodium falciparum Calcium-Dependent Protein Kinases: Opportunities for Novel Antimalarial Therapeutics* |
| P-010 | **Sampriti Ghosh**<br>SINP Kolkata | *Lanthanide-Doped Gold Nanocluster Assemblies Exhibiting Dopant-Directed Size Evolution, Symmetry-Controlled Eu3+ Emission, and Selective Chemical Recognition* |
| P-011 | **Mansi Gupta**<br>Shiv Nadar University, Delhi-NCR | *Ultrafast Hole Transport via Host–Guest Binding in Perovskite Nanocrystals: Experiment and Theory* |
| P-012 | **Injamamul Haque**<br>Presidency University, Kolkata | *Tuning Hydrogen Abstraction Reactivity of Fe(IV)=O Corrole Complexes through Local Electric Fields* |
| P-013 | **Krishna**<br>SVNIT Surat | *Interaction Mechanism in LiH-nNH3BH3 (n=1-2) Complexes: Insights from Vibrational and Chemical Shielding Analysis* |
| P-014 | **Kajal Kumbhakar** | *Enhanced Charge Transport Through Ion Networks in Highly Concentrated LiSCN-polyethylene Carbonate Solid Polymer Electrolytes* |
| P-015 | **Rimi Kundu**<br>IISER Kolkata | *Unravelling Magnesium Dependent Conformational Switching in Flaviviral RNA* |
| P-016 | **Sankar Maity**<br>NIT Rourkela | *Glucose-Mediated Stabilization of Ethanol-Stressed Lipid Bilayers: Insights from Molecular Dynamics* |
| P-017 | **Srimila Mallick**<br>IIT Guwahati | *Enhanced Inhibition of Amyloid $\beta$ Oligomerisation by a Coumarin- Chalcone Hybrid over a Coumarin Derivative* |
| P-018 | **Sourav Manna**<br>IIT Kharagpur | *Thermal and Light-Induced Catalysis in Pyridoxal 5′-Phosphate-Dependent Aspartate Aminotransferase* |
| P-019 | **Balaram Mondal**<br>IIT Guwahati | *Ligand-Specific Binding Mechanism and Dynamic Modulation of Auxin Receptor TIR1 by Structurally Diverse Auxin Analogs* |
| P-020 | **Anwesha Mukherjee**<br>University of Kalyani | *Bile salt incorporated vesicles – Modulation of their characteristics and fluorescence probing of their microenvironment* |
| P-021 | **Rik Niranjan Mukherjee**<br>SNBNCBS Kolkata | *Continuous Time Random Walk in Acetamide Deep Eutectics: Emergence of Dynamical Separation of Particles as Glass Transition is Approached* |
| P-022 | **Sutanu Mukhopadhyay**<br>SNBNCBS Kolkata | *OrFeaUs: Harmonic-Percussive Source Separation (HPSS)-based Feature Extraction from Molecular Dynamics Trajectories* |
| P-023 | **Tamisra Pal** | *Benchmarking Generative-AI-driven sampling of protein conformational landscapes* |
| P-024 | **Anuvab Panda**<br>IIT Kanpur | *Dynamical quantum chaos in one-dimensional transverse field Ising model* |
| P-025 | **Subir Podder**<br>Raiganj University | *A Novel Naphthofluorescein Derivative as an Antioxidant for Biodiesel: Integrated DFT, Molecular Dynamics, and Machine Learning Insights* |

| No. | Presenter | Title |
|---|---|---|
| P-026 | **Priya**<br>IIT Kanpur | *Green's function formalism for kinetic energy density functional for atoms.* |
| P-027 | **Madhumita Rano**<br>Ashoka University, Sonipat | *State-specific computations of vibrational and electronic excited states* |
| P-028 | **Rishu**<br>IIT Delhi | *Collective Reaction Dynamics during Ligand Exchange in Atomically Precise Metal Nanoclusters* |
| P-029 | **Saswata Roy**<br>Azim Premji University, Bengaluru | *Challenges in scalable excited state semiclassical dynamics* |
| P-030 | **Gourab Saha**<br>IACS Kolkata | *Quasiclassical Reaction Dynamics: Diels—Alder versus hetero-Diels—Alder Reactions* |
| P-031 | **Dibyamanjaree Samant**<br>IISER Kolkata | *Mapping the sgRNA-induced Cas9 conformational activation pathways integrating structure-based modeling and VAMPnet* |
| P-032 | **Arka Prava Sarkar**<br>SNBNCBS Kolkata | *Investigating the nature of anion migration in halide perovskites in presence of single layer graphene* |
| P-033 | **Mokshi Sharma**<br>Central University of Jammu | *Variational Framework for the Calculation of Vibrational States and Thermal Properties with the Effective Harmonic Oscillator* |
| P-035 | **Ananya Sinha**<br>IACS Kolkata | *Accelerating Selected Configuration Interaction with Restricted Boltzmann Machine* |
| P-036 | **Vishal Yadav**<br>IISER Kolkata | *From Cause to Consequence: Explainable AI-Guided Reaction Coordinate Reveals Thermodynamic and Kinetic Mechanisms of Nucleic Acid Base-Flipping* |

# Poster Session B

Day 2 · Thu, 29 Oct 2026 · 16:45 – 18:15 · Session 11 · Chair: Niladri Patra (IIT (ISM) Dhanbad)

| No. | Presenter | Title |
|---|---|---|
| **Invited Faculty Posters** | | 11 posters |
| IP-08 | **Barun Kumar Maity**<br>SINP Kolkata<br>abstract with SL-10 | *Specific DNA Recognition Induces Folding Transition of the Oncogenic Fusion Protein PAX3FOXO1* |
| IP-09 | **Debashree Ghosh**<br>IACS Kolkata | *Title to be announced* |
| IP-10 | **Padmaja Prasad Mishra**<br>SINP Kolkata | *Exploring Toehold-Independent DNA Strand Displacement through Parallel Triplex Formation* |
| IP-11 | **Sudip Das**<br>SINP Kolkata | *Physics-Informed Machine Learning for Enzyme Catalysis* |
| IP-12 | **Amit K. Paul**<br>Bose Institute, Kolkata | *Mode-Dependent Vibrational Energy Flow in Hydrogen-Bonded Dimers: A Unified Mechanism for Intramolecular Vibrational Energy Redistribution and Vibrational Predissociation* |
| IP-13 | **Harun Al Rasid Gazi**<br>Aliah University, Kolkata | *Decoding the Molecular Interactions of Thymol, Thymoquinone, and Lawsone with DNA and Protein: Experimental & Computational Approach* |
| IP-14 | **Rajarshi Chakrabarti**<br>IIT Bombay | *Active Polymers in Porous Media: Activity-Driven Conformational and Transport Dynamics* |
| IP-15 | **Surajit Maity**<br>IIT Hyderabad | *Quantifying the Intrinsic Energetic Thresholds of Solvent-Driven Excited-State Proton Transfer via Isotopic Tunneling Quenching* |
| IP-16 | **Tushar Kanti Mukherjee**<br>IIT Indore | *Regulation of Protease Activity of Papain via Biomolecular Condensation and Its Reactivation by L-Cysteine* |
| IP-17 | **Arijit Kumar De**<br>IISER Mohali<br>abstract with SL-08 | *Unveiling Time-Dependent Vibronic Coupling by Third- and Fifth-order Raman Spectroscopy* |
| IP-27 | **Abhijit Dan**<br>MAKAUT, West Bengal | *Interfacially Engineered Liquid Crystal Microdroplets: A Robust Platform for Label-Free Optical Biosensing* |
| **Contributed Posters** | | 35 posters |
| P-037 | **Md Asif Amin**<br>Suri Vidyasagar College | *Coronene Based Two Dimensional Metal-Organic Framework with High Spin-Filtering Efficiency* |
| P-038 | **Nidhi Arya**<br>IIT Jodhpur | *Unravelling the $Mg^{2+}$-Dependent Structural Dynamics of DNA Holliday Junctions at the Single-Molecule Level* |
| P-039 | **Indrani Bhattacharya**<br>SNBNCBS Kolkata | *Ascorbic Acid Modulates the Hydration Dynamics of Urea and Glucose: Insights from Terahertz Spectroscopy and Molecular Dynamics Simulations* |
| P-040 | **Sayari Bhattacharya**<br>SNBNCBS Kolkata | *The Fibril Tip Sets the Route, Not Just the Destination: Polymorph-Specific Kinetics of A$\beta$ 42 Monomer Incorporation* |

| No. | Presenter | Title |
|---|---|---|
| P-041 | **Sakshi Chawla**<br>IIT Gandhinagar | *Tailoring Herzberg-Teller Vibronic Interactions in Tetrapyrrole-Based Systems* |
| P-042 | **Shrestha Chowdhury**<br>SNBNCBS Kolkata | *Structural Deviations from Ideality in Alcohol + Water Azeotropes: Molecular Scale Investigations* |
| P-043 | **Kingshuk Das**<br>IACS Kolkata | *Salt-Mediated Molecular Recognition of the p53 C-terminal Domain* |
| P-044 | **Krishnandu Dey**<br>NIT Meghalaya | *Photoswitch activity of an Acyl-hydrazone dimer: A non-adiabatic dynamics study.* |
| P-045 | **Priya Dey**<br>Kyoto University, Japan | *Pepper-Mill Protein Dynamics: Decoding the Mechanism of MSPA for ssDNA Translocation* |
| P-046 | **Sk Samsul Ghaus**<br>IISER Kolkata | *Engineering HLCT-AIE Active Molecule for Efficient Flexible Optical Waveguides: Photophysics, Mechanics, and Opto-electronic Integration* |
| P-047 | **Oushnik Sen Gupta**<br>SINP Kolkata | *Monitoring enzyme activity on the surface of a self-referenced near-white light emitting assembly of atomic clusters.* |
| P-048 | **Subhabrata Hazra**<br>IACS Kolkata | *Intermediate Relaxation Timescale in Bulk Water: A Temperature-Dependent Investigation* |
| P-049 | **Tathagata Islam**<br>SINP Kolkata | *Supramolecular assembly-driven emergent chirality with simultaneous induction and ligand inversion in atomic clusters* |
| P-050 | **Vijay Kumar**<br>IIT Kharagpur | *Determinant Sampling and Subspace Diagonalization for Strongly Correlated Molecular Systems* |
| P-051 | **Subrata Kundu**<br>IIT Jodhpur | *$Mg^{2+}$-Dependent Dynamics and Kinetics of a DNA Holliday Junction Studied by Single-Molecule FRET.* |
| P-052 | **Himashree Mahanta**<br>Assam Kaziranga University | *Chemical Dynamics Simulations of Benzene-Hexachlorobenzene Complexes: Association, Ensuing Dissociation, and Comparison with Related $\pi-\pi$ Molecular Complexes* |
| P-053 | **Koushik Makhal**<br>IIT Hyderabad | *A potential gated formic acid oxidation reaction on the Rh-Cr dual-atom catalyst water interface* |
| P-054 | **Apurba Manna**<br>IIT Kharagpur | *Unravelling the Microscopic Properties of a Globular Protein in Aqueous Deep Eutectic Solutions using Molecular Simulations* |
| P-055 | **Archi Mishra**<br>NIT Karnataka, Surathkal | *Effect of membrane composition on the structural dynamics of Amyloid Precursor Protein(APP)* |
| P-056 | **Piyali Mukherjee**<br>IIT Bombay | *A Theoretical Investigation of the Encapsulation of Small Molecules within Coacervates of Elastin-like Polypeptides* |
| P-057 | **Venkatesh N**<br>IIT Patna | *Growth of Low-Density Liquid Domains Drives Fickian, Yet Non-Gaussian Diffusion in Supercooled Water* |
| P-058 | **Rishabh Kumar Pandey**<br>CUHK Shenzhen | *Vibronic Coupling Effects in the Photoelectron Spectra of LiB6-* |

| No. | Presenter | Title |
|---|---|---|
| P-059 | **Roja Satvika Puvvada**<br>GITAM University | *Unravelling the role of aqueous choline chloride-polyol deep eutectic solvents in protein stability* |
| P-060 | **Rajendra Rath**<br>NIT Rourkela | *Emergent Mixed Crowding Effect on Protein Dimerization* |
| P-061 | **Indranil Roy**<br>IISc Bengaluru | *Anisotropic quantum beats report room temperature functional vibronic couplings in light-harvesting aggregates* |
| P-062 | **Sudhriti Roy**<br>IIT Jodhpur | *Engineering Heterotypic Biomolecular Condensates with Synthetic Peptides for Controlled Spatial Organization and Liquid-like Nature* |
| P-063 | **Gourab Saha**<br>IIT Kharagpur | *Molecular Insights into the A$\beta$-42 Tetramer Induced Disruptive Effects on a Model Phospholipid Membrane* |
| P-064 | **Koushik Saha**<br>IACS Kolkata | *Quantum Dynamics and Mean Square Displacement of a Nonlinear Brownian Oscillator* |
| P-065 | **Dipayan Sarder**<br>IIT Kharagpur | *Microscopic Understanding of DNA Groove Binding by Hydrophilic and Hydrophobic Ionic Liquids* |
| P-066 | **Arghya Sen**<br>University of Rostock, Germany | *CsMnBr3 Nanocrystals: Excitation-Dependent Photophysics and Curious Case of Carrier Dynamics from Picoseconds to Microseconds* |
| P-067 | **Pallav Sengupta**<br>IIT Guwahati | *Distal residue mutations dictate substrate binding in MtbThyX* |
| P-068 | **Deepak Sharma**<br>IIT Jodhpur | *Dual Effect of RNA-like Polyelectrolytes on Stability and Dynamics of Biomolecular Condensates: A Tale of Competitive Short- and Long-Range Interactions.* |
| P-069 | **Vishnu Sudarsanan**<br>IISER Pune | *Li2 O Vacancy-Induced Modulation of Oxygen Redox in Li2MnO3 Surfaces: A First Principles Study* |
| P-105 | **Titas Kumar Mukhopadhyay**<br>NIT Jamshedpur | *Self-Assembled PTCDA Coatings on Graphene Profoundly Improve the Biocompatibility Toward Genetic Materials* |
| P-106 | **Debasish Barman**<br>Kyushu University, Japan | *Precise Control of Charge-Transfer for Triplet Harvesting: Functional Molecular Designs for High-Efficiency Narrowband TADF-OLEDs* |

# Poster Session C

Day 3 · Fri, 30 Oct 2026 · 16:55 – 18:25 · Session 17 · Chair: Debabrata Seth (IIT Patna)

| No. | Presenter | Title |
|---|---|---|
| **Invited Faculty Posters** | | 8 posters |
| IP-18 | **Bhabani S. Mallik**<br>IIT Hyderabad | *Multiscale Modeling of Electrochemical Catalysis and Energy Storage Systems via Molecular Dynamics Simulations* |
| IP-19 | **Ranjit Biswas**<br>SNBNCBS Kolkata | *Conductivity in Battery Electrolyte Systems: Impact of Ultrafast Solution Dynamics, Ion-Ion Motional Correlations, and Solution Heterogeneity* |
| IP-20 | **Suman Chakrabarty**<br>SNBNCBS Kolkata | *Navigating Pathways in Free Energy Landscape: Adaptive (Machine) Learning Strategies Towards Rare Event Kinetics* |
| IP-21 | **Souvick Biswas**<br>IISER Thiruvananthapuram | *Resonantly Stabilized Free Radical Mediated Mass Growth: Indenyl Chemistry as the Common Thread of Planar and Curved PAHs* |
| IP-22 | **Anup Ghosh**<br>Bose Institute, Kolkata | *Beyond the Sulfoxide Oxygen: NMR Spectroscopy and Machine-Learned Dynamics Reveal $\alpha$-C–H···Ow Hydrogen Bonding in Dimethyl Sulfoxide-Water* |
| IP-24 | **Padmabati Mondal**<br>IISER Tirupati | *A multiscale study in search of photoswitchable drug for serotonin receptors* |
| IP-25 | **Anirban Panda**<br>J. K. College, Purulia | *Addition Reaction Networks and Partial Ordering of Phosphorus–Sulfur Binary Compounds: A Theoretical Study* |
| IP-26 | **Subhadip Ghosh**<br>NISER Bhubaneswar | *Spatially Resolved Energy Transfer in Hexagonal Cs4PbBr6 Microdisks Revealed by Single-Particle Spectroscopy* |
| **Contributed Posters** | | 33 posters |
| P-070 | **Farhin Akhtar**<br>RGIPT Sivasagar | *Multifunctional Plasmonic Fluorescent Nanocomposites for Ultrasensitive Molecular Sensing, Antimicrobial Defense and High Resolution Bioimaging* |
| P-072 | **Anupaul Baruah**<br>Dibrugarh University | *A Light-weight Monte Carlo Simulation Based In Silico Protein Design Method for Mutation Induced Fold Switch* |
| P-073 | **Sreyan Bhowmick**<br>SNBNCBS Kolkata | *Ligand-driven entropic collapse directs mechanical strain to facilitate BirA dimerization* |
| P-074 | **Ipsita Chakraborty**<br>S. M. College, Bhagalpur | *Unravelling PNIPAM Hysteresis: A Solvent Relaxation NMR Study of the Globule-to-Coil Transition* |
| P-075 | **Samsung Raja Daimari**<br>IIT Guwahati | *Gas and Aqueous Phase Oxidation of a Series of Lactones: Initiated with OH Radicals* |
| P-076 | **Supritam Datta**<br>IIT Indore | *A Sustainable and Catalyst-Free Direct Photochemical Route for the Conversion of Amines to Imines via C–N Coupling Reaction Under Ambient Conditions* |
| P-077 | **Pradipta Dey**<br>IACS Kolkata | *Effect of Protein on Photoisomerization of Bacteriophytochrome* |

| No. | Presenter | Title |
|---|---|---|
| P-078 | **Parineeta Gogoi**<br>IISc Bengaluru | *Tailoring Quantum Dot Properties for Quantum Science: Influence of Charge, Energy Transfer and Anisotropy on Exciton Dynamics in Quantum dots and their Assemblies* |
| P-079 | **Yugant PM Guddha**<br>IIT Guwahati | *Unveiling the Influence of Biomolecules on the Relaxivity of Mn(II) Based Contrast Agents: A Molecular Dynamics Study* |
| P-080 | **Aanchal Hurmade**<br>IISc Bengaluru | *Raman Spectroscopic Investigation of Biochemical Changes in Imiquimod-Induced Psoriasis Model.* |
| P-081 | **Mira Jhawar**<br>IIT Guwahati | *From Core Insertion to Surface Binding: A Molecular Dynamics Study of hCT10-22 Fragment Behavior on Different Lipid Membranes* |
| P-082 | **Neha Kundara**<br>Shiv Nadar University, Delhi-NCR | *Investigation of the interactions of influenza A virus-encoded miRNA with human PCBP2 mRNA and Agronaute-2 protein at the single-molecule level* |
| P-083 | **Abhiroop Lahiri**<br>IACS Kolkata | *Committor-Based Detection of Post-Transition-State Bifurcations from Enhanced-Sampling Simulations* |
| P-084 | **Dibyendu Maity**<br>SNBNCBS Kolkata | *Quantitative Pathway-Resolved Kinetics from Neural Network-Guided Weighted Ensemble Simulations* |
| P-085 | **Abdul Aziz Mandal**<br>SNBNCBS Kolkata | *Mechanistic Role of Different Functional Groups in Inhibiting Tryptophan Self-Assembly: Comparison between Aromatic and Nonaromatic Hydroxyl Moiety-Rich Chemical Compounds* |
| P-086 | **Anurag Maurya**<br>IISc Bengaluru | *Stochastic Thermodynamics of a Non-Markovian Random Process* |
| P-087 | **Anandita Mitra**<br>IIT Guwahati | *Therapeutic Targeting of Cancer-Associated PKM2 Mutants by Shikonin via Mutation-Induced Pocket Recognition* |
| P-088 | **Mainak Mukherjee**<br>Sri Sathya Sai Institute of Higher Learning | *Computational Investigation of Through-Bond and Through-Space Charge Transfer for Reduced or Inverted $\Delta EST$ in TADF Emitters* |
| P-089 | **Shreya Mukherjee**<br>IIT (ISM) Dhanbad | *Estimation of Absolute Protein–DNA Binding Free Energy using Streamlined Geometric Formalism* |
| P-091 | **Somnath Paitandi**<br>IIT Guwahati | *Mg-Co-B Chemical Space for Mg-Ion Cathodes: Evolutionary Search, Machine Learning, and Chemical Bonding Analysis* |
| P-092 | **Shivam Pandey**<br>IACS Kolkata | *Turning Heat into Electricity: Driving High ZT through Soft Phonon Engineering* |
| P-093 | **Juriti Rajbangshi**<br>University of Wisconsin-Madison, USA | *Molecular Insights and Predictive Models for Solvent Selection in Lignin Valorization* |
| P-094 | **Samarth Razdan**<br>IIT Bhilai | *Molecular Engineering of Antiaromatic Orangarin-based Sensitizers for High-Performance Dye-Sensitized Solar Cell Applications* |

| No. | Presenter | Title |
|---|---|---|
| P-095 | **Roshan**<br>IIT Delhi | *Interfacial engineering of waste derived Char/VO2 composites for stable electrochemical energy storage* |
| P-096 | **Arnab Roy**<br>IACS Kolkata | *Anti-Kasha-Type Spin-Vibronic Dynamics Drive Photoinduced Ni–H Umpolung in Ni-pincer complex* |
| P-097 | **Debasish Saha**<br>IISER Bhopal | *Non-Markovian escape under stochastic resetting* |
| P-098 | **Adyasa Sahoo**<br>IIT Guwahati | *Structural Responsiveness as the Key to Water's Phase Behavior: Lessons from Machine-Learned mW and BOP Models.* |
| P-099 | **Jagori Sarkar**<br>IIT Kanpur | *Decoding the Rate Determining Step in plasmidium SHMT to Guide Antimalarial Inhibition:A QM/MM Enhanced-Sampling Free-Energy Study* |
| P-100 | **Shaheerah Shahid**<br>SNBNCBS Kolkata | *Disentangling Heterogeneous Trajectory Ensembles by an Automated and Explainable Framework for Pathway Clustering and CV Identification* |
| P-101 | **Mohd Ayaz Siddique**<br>IIT Guwahati | *Mechanistic Insights into Substrate Recognition by the Key Quorum-Sensing Regulator Protein SepM in Streptococcus mutans* |
| P-102 | **Rahul Sutradhar**<br>IACS Kolkata | *Implicating the Role of Enhanced Oxyl Attribute in Facilitating Exceptional C—H Activation by a [Co2 III,IV(μ-O)2] Diamond-Core Complex: A Theoretical Perspective* |
| P-103 | **Himanshu K. Tiwary**<br>IIT Jodhpur | *Synthesis and Characterization Study of Precursor-Controlled Multicolour Carbon Quantum Dots for Bioimaging and Drug Delivery Applications* |
| P-104 | **Sumit Singha**<br>University of North Bengal | *Engineering Nanoscale Interfaces for Enhanced Förster Resonance Energy Transfer* |

ABSTRACTS

# Oration Lectures

Sadhan Basu Oration · Mihir Chowdhury Oration

2 abstracts

# Nonlinear Vibrational Spectroscopic Calculations of the Dynamics of Aqueous Solutions at Charged Interfaces

Amalendu Chandra*

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We will discuss second and fourth order vibrational spectroscopic calculations of aqueous ionic solutions at charged interfaces, with emphasis on understanding the dynamics of Stern and diffuse electrical double layers at the interfaces. Specifically, we will discuss results of our recent work on aqueous interfacial systems of sodium dodecyl sulfate monolayer in the presence of chloride salts of mono and divalent countercations. The spectral diffusion of interfacial water is investigated through calculations of two-dimensional vibrational sum-frequency generation (2D-VSFG) spectroscopy[1,2] and kinetics of hydrogen-bonds and escape processes of water from headgroup solvation shells. The current study[3] reveals five distinct characteristic timescales governing interfacial water dynamics: Inertial motion, H-bond stretching and librations without breaking, transient and true hydrogen bond breaking, and the residence time of water molecules in the solvation shells of surfactant headgroups. The dynamics of diffuse double layers is extracted through calculations of the difference 2D-VSFG of concentrated solutions over that of dilute solutions.

**References**

[1] S. Nihonyanagi, J. A. Mondal, S. Yamaguchi, and T. Tahara, *Annu. Rev. Phys. Chem.* **64**, 579 (2013).
[2] R. Malik, A. Chandra, B. Das, and A. Chandra, *J. Phys. Chem. B.* **127**, 10880 (2023).
[3] R. Malik and A. Chandra, J. Phys. Chem. B **130**, 8744 (2026), R. Malik, A. Negi and A. Chandra, to be published.

Keywords: Vibrational sum frequency generation spectroscopy; Charged interfaces, Aqueous ionic solutions, Sodium dodecyl sulfate

# Mass Spectrometry in Physical Chemistry Research

Tapas Chakraborty*, Piyali Chatterjee[1] and Megha Agarwal[2]
[1]*School of Applied Sciences and Humanities, Haldia Institute of Technology, PIN 721657, India*
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**Abstract:**

Mass spectrometry is the field of research that involves mass-to-charge ratio (m/z) measurements of atomic, molecular and cluster ions in the gas phase, and used primarily as a powerful analytical technique in all areas of science and technology since the beginning of the twentieth century. From analytical viewpoints, although the technique is used for identification and quantification of molecular species in a mixture, physical chemists leveraged the technique for the determinations of molecular structure, thermodynamic properties, and reaction dynamics at an absolute molecular level. While molecular spectroscopy, over a wider range of electromagnetic spectrum, has traditionally served as a versatile and non-invasive method for elucidation of intrinsic molecular structures, but as the molecular size is increased, structure determination by spectroscopy is constrained by isomeric distributions and their interconversions over low energy barriers, spectral congestion due to thermal broadening, and the inherent limitations of the lack of mass selectivity. In recent years, mobility mass spectrometry has emerged as a complementary tool to reveal much of the features of molecular structures, particularly for complex molecular systems in the gas phase. In my talk, experimental data from recent studies performed in our group at IACS Kolkata in this area of mass spectrometry will be presented. Integration of high-performance liquid chromatography with collision induced dissociations at variable collisional energies of the mass-selected molecular species allows extractions of information with a fairly high degree of accuracy. As elucidatory archetypes, I shall present data on the dimeric complexes of polypeptides, and host-guest type complexes of cyclodextrin with curcumin, which have been studied by optical methods for long[1-3].

**References:**

[1] M. Agarwal, P. Chatterjee, T. Chakraborty, *Phys. Chem. Chem. Phys.*, 2025, 27, 13939-13951
[2] P. Chatterjee, S. S. Datta, M. Agarwal, S. Dey and T. Chakraborty, *JPCA,* 2024, 128, 548
[3] P Chatterjee, S. S. Dutta and T. Chakraborty, *J. Phys Chem* A, **2022**, 126, 1591.

**Keywords:** Molecular Structure, Mass Spectroscopy, Ion Mobility, Inclusion Complex, Peptides

ABSTRACTS

# Invited Lectures

Codes IL and SL, as in the programme

59 abstracts

# Is the distance between two atoms enough to conclude about bonding?

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Chemists and biologists have used often the distance between two atoms to conclude about whether or not they are bound. This led Pauling to define and propose atomic radii, ionic radii, covalent radii and metallic radii for most atoms. These radii were useful in predicting the bond length between two atoms having ionic/covalent/metallic bond between them. While this worked reasonably well for bonding within molecules, for intermolecular bonding such as the most important hydrogen bonding, the consensus was that a radius could not be defined. Instead, the distance between X and Y or more recently H and Y in an X-H···Y hydrogen bond was compared to the sum of the respective van der Waals radii to conclude about the presence of a hydrogen bond. We showed that a hydrogen bond radius could be defined to provide a reasonable estimate of distance between H and Y in a hydrogen bonded system. A recent review discusses the evolution of hydrogen bond radius for donors and acceptors [1]. However, in a recent work, we showed that the radii could vary depending on the ∠XHY angle [2]. In 2009, we proposed a dynamic criterion for a hydrogen bond based on the zero point energy along the torsional vibrational coordinate and the barrier for torsion [3]. This emphasized the importance of including the dynamics in deciding about bonding between two molecules. Recently, in collaboration with computational data scientists, a dynamic criterion has been introduced to conclude about bonding between two atoms and identification of specific species in molecular dynamics simulations [4]. This talk will summarize our efforts in identifying a bond between two atoms in a molecule / weakly bound complex / condensed phase.

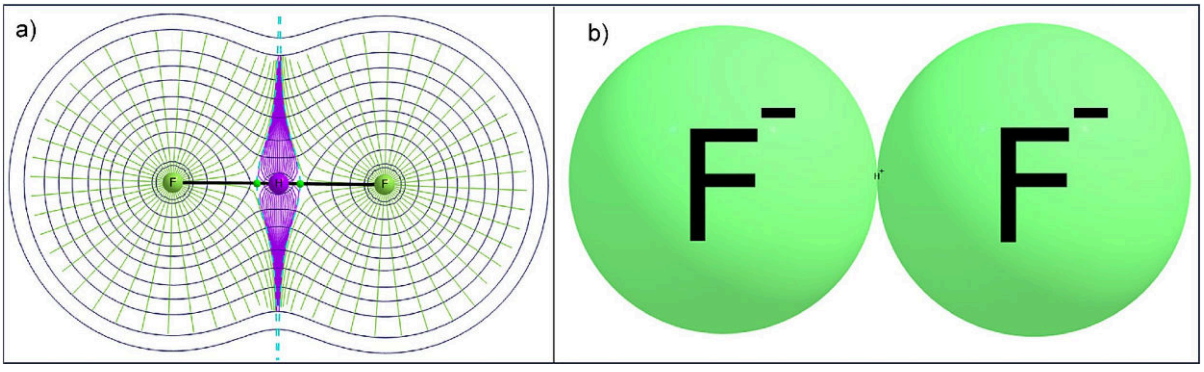



**Figure 1.** The structure of $[FHF]^-$ deduced by our work [1] on left and by Pauling [5] on right.

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**Keywords:** hydrogen bond radius, van der Waals radius, dynamics, simulation

# Beyond Crystallization Frustration: Structure and Dynamics in Model Glass Former

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The stability of a glassy system is often associated with its degree of frustration against crystallization. Understanding the glass-forming ability of a system therefore requires understanding the microscopic origins of its resistance to crystallization. A central and extensively debated question in glass physics is whether a single growing static length scale fundamentally controls the emergence of slow glassy dynamics. It has been proposed that in systems with weaker frustration, static and dynamic length scales grow together, whereas in strongly frustrated systems, these length scales may decouple. The well-known Kob–Andersen binary Lennard-Jones (KALJ) system is generally considered to belong to the latter category. We show that, despite its strong frustration against crystallization, the KALJ system exhibits a tendency toward the formation of FCC-like crystalline order [1]. We further show that a recently developed structural order parameter, which is agnostic to the system's crystallization tendency, reveals a static length scale that grows concomitantly with the dynamical length scale [2]. Finally, using unsupervised machine-learning techniques, we identify structural signatures associated with the crystallization tendency of the KALJ system, providing further support for our earlier findings. Interestingly, the order parameter emerging from the machine-learning analysis, which is directly related to the crystallization process, exhibits a strong correlation with dynamics and also displays a growing characteristic length scale [3]. Together, these results suggest that the relationship between frustration, crystallization tendency, static structural order, and glassy dynamics may be more subtle.

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**Keywords:** Supercooled liquid : Lengthscale : Machine Learning

# Generalizing Physics-based Machine Learning for prediction of hydration free energies

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The role of water in chemistry and biology cannot be overemphasized. One important quantity to understand the effect of water on solutes is the Hydration free energy (HFE). Hence, experiments and calculations for HFE play a prominent role in understanding solute-water interaction. Among different ways to calculate HFE, Machine Learning (ML) models have become quite popular, along with the more traditional statistical mechanics-based models, primarily due to speed. However, ML models often suffer from a lack of interpretation and transferability. In the ML model for HFE, under development in our group, we have used physics-based descriptors for interpretability and have recently developed a technique to treat out-of-distribution data, leading to generalization of the model. These improvements have made our model among the most accurate models for HFE calculations for small molecules.

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**Keywords:** Hydration Free Energy; Machine Leaning modelling; Out-of-distribution data

# From Surface Chemistry to Excited-State Reactivity: Unraveling Catalysis in Mono- and Bimetallic Nanoclusters

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Metal nanoclusters (NCs), owing to their atomically precise structures, discrete electronic states, and highly tunable surface chemistry, offer unique opportunities for understanding and controlling catalytic processes [1]. This talk will highlight our recent studies on the ground- and excited-state reactivity of mono- and bimetallic nanoclusters, focusing on the interplay between metal composition, surface ligands, photophysical properties, and catalytic performances. In the ground state, nanoclusters are explored for surface-controlled reactions, including enzyme inhibition, where cluster-substrate interactions and surface ligands play a critical role in molecular recognition and reactivity [2]. Bimetallic systems further provide opportunities to tune electronic structure and generate distinct catalytic sites. In the excited state, the rich photophysics of nanoclusters is exploited for light-driven redox processes and organic transformations [3]. Steady-state and time-resolved spectroscopic investigations, particularly ultrafast transient absorption spectroscopy (TAS), are employed to unravel charge-transfer pathways, excited-state lifetimes, and the formation of catalytically relevant charge-separated states.

A major focus will be the role of surface ligands, which can regulate electronic structure, substrate binding, charge transfer, and reaction pathways. By correlating metal composition, ligand environment, photophysical dynamics, and catalytic activity, these studies have established a mechanistic framework for designing nanoclusters as versatile platforms for chemical transformations.

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**Keywords:** Metal nanoclusters; Aqueous media; Ultrafast processes; Charge transfer; Catalytic activity.

# What nonequilibrium work theorems tell us about carbohydrate mechanics

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The problem of mechanical stretching of an oligosaccharide to estimate the inherent resistance and the associated free-energy change is pertinent at present, given the advent of newer polysaccharide-based materials intending to replace the conventional synthetic polymers. Unlike proteins and nucleic acids, the absence of specific structural orders in polysaccharides often introduces the element of irreversibility in the act of stretching the latter. This makes the estimation of free energy from steered molecular dynamics simulations significantly challenging, as attaining a converged data set becomes difficult. Jarzynski equality with an incomplete $\gamma$ function estimator is found to be suitable for such systems. The free-energy changes in such cases are influenced by a variety of structural attributes like the anomeric nature of the monomer and the glycosidic linkages present. This discussion will focus on how the atomic scale details of a polysaccharide destines the overall mechanical attributes of such polymers.

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**Keywords:** Jarzynski equality, mechanics, polysaccharides, glycosidic linkage, steered molecular dynamics

# TADF-Enabled Triplet Exciton Harvesting in Novel Organic Multi-functional Luminogens

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Efficient triplet-exciton harvesting through thermally activated delayed fluorescence (TADF) provides a powerful strategy for developing next-generation organic luminogens and optoelectronic materials. This talk presents complementary molecular and solid-state design strategies involving regioisomeric tuning,[1,3] steric modulation,[2] structure-packing-property engineering,[1-3] and suppression of excited-state structural reorganization[4] for the development of efficient and multifunctional organic TADF emitters.

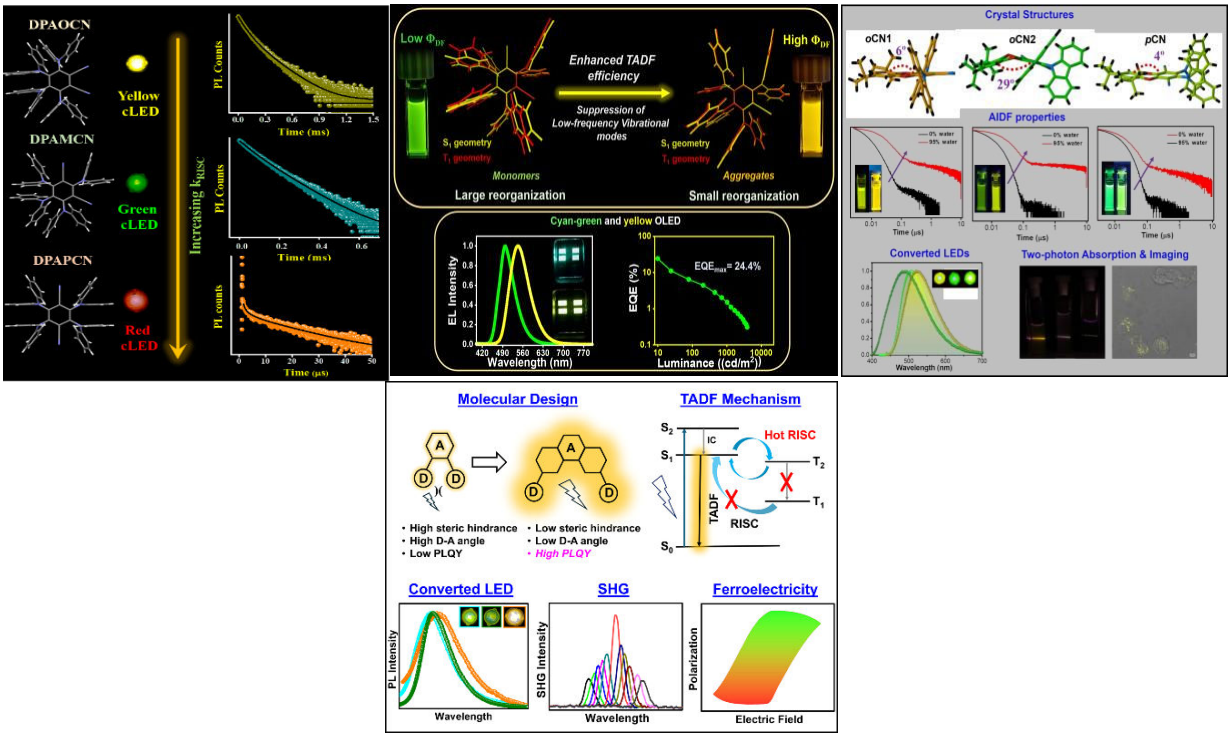



**Figure 1.** Depicts the regioisomeric (left panel), excited state structural reorganization (middle panel), crystal packing (top right panel) and steric engineering (lower middle panel) approaches for the modulation of TADF property.

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**Keywords:** Thermally activated delayed fluorescence (TADF); Organic light-emitting diodes (OLEDs); Reverse intersystem crossing; Steric modulation; Excited-state structural reorganization.

# Shedding Light on the Mechanism of Highly Selective Toluene Photo-oxidation under Nano-Confinement

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Over the past two decades, host–guest chemistry has moved beyond the mundane use of non-covalent interactions in catalysis. Photoexcitation is now known to promote charge transfer between the guest and host, enabling unprecedented photochemical reactivity. Nano-confinement offers unique opportunities for highly selective hydrocarbon oxidation through photon-enabled, charge-transfer-triggered C–H activation [1-3]. However, the mechanistic basis of these processes remains elusive till date. Using a range of excited-state theoretical methods, we have mapped the full mechanistic pathway of these photocatalytic oxidation reactions [4]. In this talk, I will highlight the key photochemical and chemical events that complete the photocatalytic cycle.

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**Keywords:** Charge-transfer, Excited States, Host-Guest, PCET, Conical Intersections

# $CO_2$ Adsorption in Humid COFs: A Transition Matrix Monte Carlo Study

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Understanding $CO_2$ adsorption in the presence of water is crucial for developing COFs for carbon capture under realistic humid conditions. In this work, we employ NVT-based Grand Canonical Monte Carlo with Transition Matrix Monte Carlo (TMMC) to investigate $CO_2$ adsorption in a COF under humid conditions. Initial simulations have successfully reproduced the $CO_2$ adsorption isotherm, and ongoing simulations are being extended to $CO_2$–$H_2O$ coadsorption. We aim to elucidate the influence of water on $CO_2$ uptake and identify the molecular-level adsorption sites and interactions governing competitive or preferential adsorption. The study will provide molecular insights into $CO_2$ capture in COFs under humid environments and complement experimental observations.

**Keywords:** three to five keywords, separated by semicolons

# Learning Transferable Collective Variables For Ligand Binding Transition Through Explainable Machine Learning

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Choosing appropriate collective variable for bio-molecular processes is a challenging task. Moreover, while constructing the free energy landscape, solvent degree of freedom is often neglected. 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 in conjucture with explainable AI algorithm Shapley Additive exPlanation (SHAP) in polymer collapse transition. Using this protocol, we have shown that hydration water is the most crucial order parameter which dictates the major barrier. Next, we have combined this protocol with Well-Tempered Metadynamics to accelerate the collapse transition in different lengths of polymer systems. It was found that incorporating transition state ensembles knowledge drastically improves the sampling in these polymer systems and achieves faster convergence in free energy profiles.

We extend this protocol in accelerating drug binding in various protein-ligand complexes. Intriguingly, it was found that ligand solvation plays most dominant role in driving ligand binding transition. Using this developed protocol, the optimized CV achieves faster free energy convergence. The estimated binding free energy and kinetics matches reasonably well with that of experimental values. We have also shown that the CV is transferable across diverse protein-ligand complexes which bypass the extensive training data requirements for constructing optimized CV. Moreover, we also developed a method to explore free energy landscapes and identify all possible binding pockets through a blind exploration approach where binding site information is not used. This blind exploration method successfully predicts experimental binding free energy and can be used in therapeutic drug design.

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# Power-law scaling of depth of the potential wells in bistable systems

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Depth of the potential wells play a critical role in fluctuation assisted rate processes in variety of chemical, physical and biological systems. However in multidimensional dynamical systems determination of potential landscape and the depth of the wells is a challenging task due to lack of general definition of pseudo-potential energy in these systems. Although dynamical systems theory have been proven to be quite useful in understanding biological phenomena involving transitions between two or more states, however a connection between the dynamical systems and potential landscape is lacking. We show that, in bistable systems, the depth of the wells follow power-law scaling with the size of basins of attraction determined from bifurcation diagrams of the dynamical systems. The scaling exponents originating from saddle-node and pitchfork bistability are ~2.85 and ~4.0, respectively. Importantly the scaling behaviour and the exponents are independent of the mechanistic details of the models and the parameters indicating scaling universality. The scaling laws provide a route to determine the depth wells from the bifurcation diagrams bypassing the challenging task of direct calculation of pseudo-potential energy in multidimensional dynamical systems.

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**Keywords:** Dynamical systems, potential well, bistability, power-law scaling, bifurcation

# Free Energy and Kinetics of Unbinding of Enzyme Inhibitors

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Abstract

Classical molecular dynamics simulations are performed on the enzymes, human carbonic anhydrase II (HCA II) and bovine pancreatic ribonuclease A (RNase A), in the presence of small organic molecules that are known to have varying inhibitory properties towards the chosen enzymes. Several unbinding pathways are detected in each case with multiple free energy basins corresponding to a wide range of bound, surface-bound and unbound states of the inhibitors characterized by a non-uniform distribution of unbinding rates from these states. We also highlight how a non-trivial conformation dependence may result in a large variation of residence times of some inhibitors at the active site of RNase A.

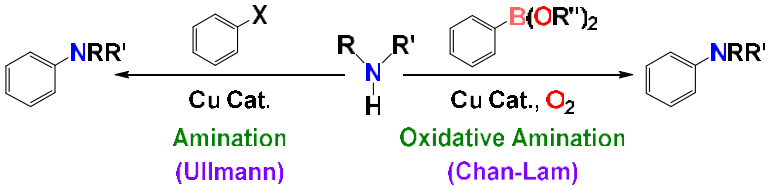
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# *In Silico* mechanistic rationalization of Copper-complex catalyzed oxidative reactions

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Methodology for carbon-nitrogen (C–N) bond formation is an active field of research for organic synthesis because nitrogen containing compounds are necessary building scaffolds for useful pharmacophores and bioactive compounds.[1] Transition metal-catalyzed C–N cross-couplings are broadly based under two sections: the classical nucleophile-electrophile coupling characterized by the Ullmann-Goldberg reaction and the oxidative nucleophile-nucleophile coupling, the Chan-Evans-Lam (CEL) amination as represented in Scheme 1.[2,3] The current presentation will discuss a detailed mechanistic investigation, employing the state-of-the-art quantum mechanical calculations, of the C–N and C–O bond formation reactions within the $Cu^{II}$ catalyzed CEL protocol.[4] The calculations will broadly provide an overview of the following fundamental steps in the catalytic transformation: catalyst activation, transmetalation, disproportionation, reductive elimination and finally oxidation to generate the monomeric $Cu^{II}$ catalyst.[4] Furthermore, the role of transmetalated byproduct $B(OH)_3$ in circumventing the use of additional base will also be discussed. The modified protocol shows enhanced efficiencies towards amination and etherification reactions in presence of less effective aryl boronic acid pinacol esters.[3]




**Scheme 1.** Copper catalyzed C–N cross-coupling reaction.

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**Keywords:** Copper catalysis; mechanisms; DFT; ligand design; carbon-heteroatom bond formation, regioselectivity

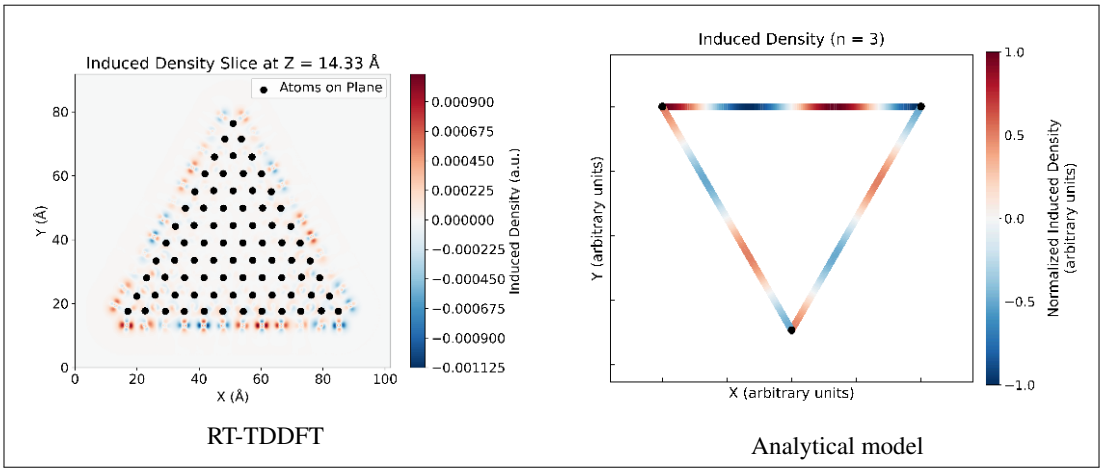
# An analytical hydrodynamic model for coupled edge plasmons in TMD nanoflakes

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Plasmonic near-field enhancement enables applications such as Raman spectroscopy, sensing, and hot-carrier transfer. Two-dimensional transition-metal dichalcogenide (TMD) nanoflakes host an edge-localized variant of this collective response — edge plasmons, confined to their one-dimensional metallic edges. However, these have so far been characterized largely through case-by-case real-time time-dependent density functional theory (RT-TDDFT) simulations, which are quantitatively accurate but offer insight into the underlying mode structure and dispersion only *a posteriori*. We complement this picture with an analytical hydrodynamic model that treats the conduction electrons at each metallic edge as a compressible charged fluid within a nonlocal Thomas–Fermi framework, yielding closed-form edge-plasmon eigenmodes, dispersion, and a symmetry-based selection rule under broadband excitation. Extending this picture to the three coupled edges of an equilateral triangular flake yields an effective coupled-oscillator model with explicit net-dipole and zero-dipole collective eigenmodes, along with their polarization-dependent excitation patterns. Comparison with RT-TDDFT simulations on triangular $WSe_2/MoSe_2$ nanoflakes shows that, once fitted to the fundamental edge-plasmon energies, the model reproduces the induced charge densities, relative mode amplitudes, and damping constants, and predicts higher-order edge-plasmon energies and edge-length scaling trends with good accuracy. The same framework anticipates the existence and spatial signature of a charge-transfer-plasmon-like mode at the sub-nanometre vertex, subsequently identified in the first-principles data. This minimal, mode-resolved description offers a physically transparent bridge between first-principles simulation and plasmonic design, enabling rapid interpretation of edge-dominated spectra in coupled low-dimensional nanostructures.




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**Keywords:** edge plasmons; nonlocal hydrodynamic model; transition-metal dichalcogenides; RT-TDDFT; charge-transfer plasmon

# Rheology of Block Copolymeric Ring Polymers in Dilute Solutions

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Delhi-110007.

A ring polymer is formed by joining the free ends of a linear polymer. Many biopolymers such as DNA, lipids, polysaccharides, and polypeptides exist in nature as rings. Ring polymers in different solution conditions may be an excellent model system for exploring the properties, interactions, packing and dynamics of these circular biomolecules. The ring block copolymer is composed of two different types of monomers represented by beads of different sizes and friction coefficients that are connected by harmonic springs. The intramolecular relaxation dynamics of ring block copolymers and alternating copolymers are investigated via a multiresolution bead spring model formulated within the framework of optimized Rouse-Zimm theory. The viscoelastic properties of these ring block copolymers are evaluated from the relaxation rates of their respective normal modes. The relaxation dynamics of ring block copolymers are enhanced and retarded in the low and high frequency regime, respectively, with an increase in the monomeric block length. The storage modulus of both ring diblock and ring alternating copolymers show a quasi-plateau regime demonstrating a viscoelastic solid like response of the polymer, while the loss modulus exhibits a bimodal trend due to a difference in the mobilities of the monomers of different sizes, unlike that of ring homopolymers and multiblock copolymers. The characteristic overall relaxation time of ring alternating copolymers is lower than that of ring diblock copolymers indicating a slower dynamics that spans over different time scales.

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# What is the electronic character evolution in singlet fission dimers ?

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Singlet fission refers to the spin-allowed internal conversion of an optically excited singlet into a spin-entangled triplet-pair state $^1(TT_1)$, which can subsequently decorrelate, via spin-polarized high-spin states, into two free triplets. The high-spin states are of interest for spin-polarized qubits in quantum information and sensing, while their subsequent decorrelation into triplets offers an interesting approach to photovoltaics. The rapidly expanding chemical space of synthetically tunable singlet fission templates suggest that $^1(TT_1)$ decorrelation is governed by a subtle but poorly understood interplay of molecular motifs, geometry and structural fluctuations. In particular, THz structural fluctuations in conformationally flexible singlet fission systems have been proposed to play a functional role in reducing the exchange couplings within the triplet-pair thereby driving $^1(TT_1)$decorrelation. However, probing $^1(TT_1)$evolution has traditionally relied on techniques such as microsecond EPR measurements which track spin evolution on microsecond timescales. In this talk, I will establish tracking electronic evolution via polarization-control as a complementary optical probe for probing $^1(TT_1)$decorrelation on timescales not accessible to conventional EPR.

I will first introduce our recent theoretical framework [1,2] and its experimental realization [3] for isolating the dynamics of orthogonally polarized transitions via polarization-controlled two-dimensional electronic spectroscopy (2DES, Fig. 1a,b). I will then present an extension [4] of this approach to singlet fission. Using a library of conformationally flexible pentacenic iSF dimers with varying bridging units, we show that the $^1(TT_1)$ state maintains persistent singlet-triplet electronic mixing throughout its lifetime. THz structural fluctuations and variations in bridge electronic structure, spanning conjugation, aromaticity, dihedral angles and spacer length, have little influence on diminishing the singlet electronic character. Instead, bridge connectivity exerts the dominant influence on the electronic structure of the resulting $^1(TT_1)$ state. Our observations suggest that the mechanism of triplet-pair decorrelation via THz motions operates on timescales exceeding the rotational diffusion of molecules in solution and is outcompeted by the decay of $^1(TT_1)$ to the ground state. Persistent singlet-triplet admixtures likely promote this rapid decay.

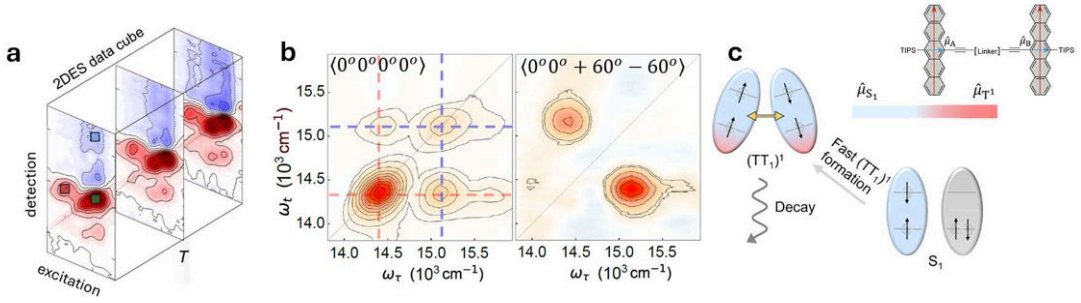



**Figure 1.** (a) Two-dimensional electronic spectroscopy (2DES) data cube with polarization-control can optically track the evolution of $^1(TT_1)$ state in singlet fission dimers, revealing persistent singlet-triplet electronic character throughout its lifetime.

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**Keywords:** two-dimensional electronic spectroscopy; polarization anisotropy; singlet fission

# β-Turn Peptides: Bridging Molecular Structure and Functional Materials

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The molecular structure of a peptide is encoded by its sequence, and subtle changes in sequence can profoundly alter its conformation and the properties of its assemblies. Understanding how sequence controls peptide folding is, therefore, an important step toward establishing molecular design principles for functional peptide materials. Our studies on capped $^{D}$Pro-Gly containing peptides reveal how intrinsic residue propensities, backbone hydrogen bonding, and environmental effects govern secondary structure formation.[1] A combination of gas-phase and solution-phase spectroscopy, two-dimensional NMR, single-crystal X-ray diffraction, and quantum-chemical calculations shows that tripeptides with $^{D}$Pro-Gly sequence strongly promote β-turn formation, whereas subtle changes in the third-residue side chain can shift the conformational preference toward extended β-strand-like structures.[2-4] These results establish how intrinsic molecular properties and external environments, such as solvation and crystal packing regulate peptide secondary structure. This control over peptide conformation provides a molecular basis for understanding how specific secondary structures can be translated into functional supramolecular assemblies. In particular, the defined geometry and directional organization of β-turns can influence molecular packing and dipole arrangement, providing a pathway from peptide folding to macroscopic polarization. In the $^{D}$Pro-Leu ($^{D}$PL) system, a type II′ β-turn directs non-centrosymmetric molecular organization and cooperative dipole alignment, giving rise to strong piezoelectricity, ferroelectricity, and second-harmonic generation. $^{D}$PL based devices function as efficient mechanical energy harvesters, exhibiting performance among the highest reported for biomaterial-based systems, thereby underscoring their potential in bioelectronic applications.[5] Pronounced second-harmonic-generation circular dichroism of $^{D}$PL further demonstrates how molecular asymmetry can be translated into nonlinear optical functionality. Thus, the progression from sequence-dependent folding to β-turn formation, supramolecular organization, and macroscopic function provides a framework for rationally designing biocompatible peptide materials with programmable electromechanical and nonlinear optical properties. Beyond their fundamental role in peptide folding, β-turns can therefore serve as molecular building blocks for functional materials and emerging bioelectronic technologies.

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**Keywords:** β-Turn peptides; Peptide folding; Structure-function relationship; Piezoelectricity; Bioelectronic materials

# Memory Effects and Ruggedness as Microscopic Sources of Internal Friction in Chemical and Biophysical Dynamics

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Barrier-crossing rates in biophysical systems often deviate from the inverse viscosity dependence predicted by Kramers theory. This fractional viscosity dependence is commonly attributed to internal friction, but the molecular origins of this phenomenon remain debated, with proposed mechanisms including specific intramolecular interactions and rugged free-energy landscapes [1]. Here, we investigate the microscopic origins of anomalous viscosity dependence using molecular dynamics simulations spanning simple model systems, small molecules, and proteins.

We show that **memory effects arising from the delayed response of degrees of freedom [2] coupled to the reaction coordinate** can produce fractional viscosity dependence without invoking an additional phenomenological friction term. This mechanism is demonstrated in model systems and butane dihedral rotation [3,4], and extended to protein dynamics through the ring flipping of a buried residue in cytochrome *c* [5] and fluorescence-lifetime switching in eGFP. Across these systems, the molecular origins of memory vary from solute–solvent coupling to coupling between internal degrees of freedom within the protein.

We further demonstrate that **free-energy landscape ruggedness** can produce anomalous viscosity dependence through a fundamentally different mechanism: additional residence time in metastable microbasins modifies the kinetics without requiring memory-dependent friction.

Together, these results demonstrate that fractional viscosity dependence is **not a unique signature of a single molecular mechanism**, and highlight memory effects and landscape ruggedness as distinct microscopic origins of the phenomenon commonly described as internal friction.

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**Keywords:** Internal Friction, Rugged Landscape, Dynamical Recrossing, Enhanced Simulation

# Does Excitation Energy Transfer Happen in Doped Perovskite Nanocrystal?

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Doped all inorganic perovskite-nanocrystal (PNC) has many advantages in comparison to the corresponding undoped one, in terms of fundamental as well as applications points of view.[1-3] A typical of such a system is Mn doped $CsPbCl_3$ or $CsPb(Cl/Br)_3$ PNC.[4-5] Triply degenerate $Mn^{2+}$ excited state ($^4T_1$) is much lower in energy than the conduction band minimum of the host $CsPb(Cl/Br)_3$ PNC.[5-6] In this Mn doped PNC, both host and dopant PL emission are observed, the intensity of the former band being lower than that of the latter band.[4] Does "excitation energy transfer" (EET) happen between the host and dopant? Although at the ensemble level some superficial signatures of EET are observed, however, at the ultrasensitive single particle level, no specific signature of EET is observed. In literature, several reports are there showing EET between the host band of undoped PNC as the donor and an external organic dye as acceptor.[7-10] However, there is hardly any report of EET employing dopant emission band of PNC and an external organic dye. Is it possible that EET will happen between dopant as the donor and the organic dye as an acceptor? If possible, then what kind of mechanism operates for the EET phenomenon?

Detailed results based on structural and dynamical analyses will be put forward to answer these important questions.

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**Keywords:** Doped Perovskite Nanocrystal; Excitation Energy Transfer (EET); Structural & Dynamical Analyses; Single Particle Spectroscopy; Mechanism of EET.

# Ions as Molecular Architects Shaping RNA Folding

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The conventional picture often portrays ribosomal RNA often as highly structured, while messenger RNA and many other RNAs are imagined as extended, flexible, or even "limp spaghetti". But is this distinction supported by an absence of structure, or does it partly reflect how we have historically thought—and talked—about RNA? As provocatively discussed by Vicens and Kieft in *Thoughts on how to think (and talk) about RNA structure* [1], with an ever-growing repertoire of RNA structures being resolved—and many more yet to be characterized—RNA may be better understood not through a simple structured–unstructured dichotomy, but as a dynamic ensemble of interconverting conformations. For a highly charged molecule such as RNA, this ensemble is inseparable from its ionic environment [2]. Ions not only screen electrostatic repulsion but can differentially stabilize conformational states through localized ion-coordination [3,4]. Capturing this coupling is challenging: For instance, $Mg^{2+}$ ion-coordination exchange between hydrated outer-sphere and directly coordinated inner-sphere states involves a substantial free-energy barrier, making repeated ion-coordination exchange together with RNA conformational transitions difficult to sample using conventional explicit-solvent molecular dynamics [5]. Addressing this limitation, we developed the Structural Topology-Based Electrostatics Model (STEM) to bridge these scales by combining implicit monovalent-ion screening with explicit $Mg^{2+}$ capable of dynamic outer-/inner-sphere coordination exchange [6]. STEM reproduces experimental ion-interaction coefficients, SAXS-derived RNA compaction, and crystallographic $Mg^{2+}$ coordination sites. In a 58-nucleotide rRNA, STEM resolves intermediate and native ensembles and reveals how localized $Mg^{2+}$ coordination is coupled to tertiary folding and conformational breathing. These results suggest that ions do more than stabilize a pre-existing RNA structure: ion-coordination dynamics can redistribute conformational populations and reshape the folding free-energy landscape. If the ionic atmosphere is an integral part of what defines an RNA structural ensemble, then attempting to predict RNA structure without accounting for it risks solving RNA folding problem.

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**Keywords:** RNA Structure, dynamic conformations, folding free-energy landscape, Ion-coordination

# From Conformer Resolution to Bond Scission: An Integrated Approach Using REMPI, RIDIR, and VCD/ECD Spectroscopy

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Flexible molecules or molecular complexes in the gas phase often exist as a distribution of conformers, leading to significant spectral congestion in Resonance-Enhanced Multiphoton Ionization (REMPI) and Resonant Ion-dip Infrared (RIDIR) spectroscopy.[1] This congestion, compounded by factors like short excited-state lifetimes and strong vibrational coupling, makes the assignment of specific spectral features to individual conformers virtually impossible, even when using deconvolution techniques such as fitting with Voigt profiles. The combination of Electronic Circular Dichroism (ECD) and Vibrational Circular Dichroism (VCD) with REMPI and RIDIR offers an alternative approach to overcome this challenge. The computational studies show that this integration is highly effective because ECD and VCD spectra provide distinct, sign-sensitive spectral shapes for different conformers, even when their underlying electronic or vibrational transitions are nearly degenerate.

This presentation will detail our efforts in applying this combined chiroptical approach to assign and characterize the unique, chirality-induced conformations of molecules and molecular clusters, including the neurotransmitter precursor tryptamine and the para-cresol-dimethyldisulfide complexes.[2,3]

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**Keywords:** REMPI: RIDIR: VCD: ECD: VMI

# Modified Interfacial Environment around Biomolecules in Aqueous Ionic Liquid Mixtures

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Structural stabilities and activities of biomolecular systems, such as proteins, nucleic acids, phospholipid membranes, etc. are known to be sensitive to the presence of ionic liquids (ILs) as co-solvents in aqueous environment. To obtain a microscopic understanding of the mechanism of action of ILs on different biomolecules, it is important to elucidate biomolecule-IL interaction and probe the modified interfacial environment around those in binary water-IL mixtures. We have carried out extensive molecular dynamics (MD) simulations of proteins in aqueous IL mixtures [1-3]. Preferential distribution of the IL components at the interface and their non-uniform influence on the interfacial properties have been explored in detail. Attempts have also been made to characterize the effects of ILs on the structure, stability and interfacial properties of different forms of DNA [4] and model phospholipid membranes [5]. Some important findings originating from our studies will be presented.

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**Key words**: ***Biomolecules, Ionic liquids, Molecular simulation, Interface***

# Understanding the coil-globule transition in semi-flexible polymers from an energy landscape perspective

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Despite its fundamental importance in polymer physics and protein folding, a unified understanding of the coil–globule phase transition that integrates experimental observations with theoretical models remains elusive, particularly in the critical transition regime [1, 2]. Here, we employ temperature replica exchange molecular dynamics simulations to systematically investigate this transition using a bead–spring polymer model. We explore how chain stiffness, and the strength of non-bonded interactions tune the conformational phase diagram and influence the character of the phase transition. Consistent with Flory theory, we find that at low temperatures and high interaction strengths the polymer chain adopts globule-like conformations, whereas random-coil structures are favored at high temperatures and weaker interaction strengths. In the vicinity of the phase transition, globular and random-coil structures are found to coexist. Using inherent structure formalism [3, 4], originally proposed in the context of liquid state theory, we investigate how the competition between chain stiffness and non-bonded interactions modulate the ruggedness of the energy landscape, basin anharmonicity and configurational entropy.

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**Keywords**: coil-globule transition; semi-flexible polymer; replica-exchange MD; inherent structure; energy landscape

## Atmospheric Oxidation Kinetics of Emerging Halogenated Oxygenated Volatile Organic Compounds (XOVOCs)

Halogenated oxygenated volatile organic compounds (XOVOCs) can emerge as secondary degradation products during the atmospheric oxidation of hydrofluoroethers (HFEs) and other halogenated VOCs.[1,2] We have studied the oxidation kinetics of two key classes of halogenated OVOCs: Fluoroalkyl fluoroformates (FC(O)OX, X = $CHF_2$, $CH_2F$, $CH_3$, $CH_2CF_3$) and XC(O)H/XC(O)OH (X = F, Cl, Br, and I). We have examined hydrogen-abstraction reactions with atmospheric oxidants such as OH radicals and Cl atoms using M06-2X and MP2 methods with aug-cc-pVTZ for (F, Cl, and Br) and aug-cc-pVTZ-PP (for I) basis sets for geometry optimization and thermochemistry calculations.[3] CCSD(T)-based methods were employed with aug-cc-pVXZ and aug-cc-pVXZ-PP (X=D, T, and Q) basis sets for single-point energies with complete-basis-set extrapolation.[4,5] Reaction pathways and potential-energy surfaces were mapped, and temperature-dependent rate coefficients were determined using canonical variational transition-state theory with small-curvature tunneling (CVT/SCT) and zero-curvature tunneling (CVT/ZCT). The kinetic data obtained were used to estimate atmospheric lifetimes and evaluate atmospheric impact parameters of these compounds. This integrated computational study provides valuable mechanistic and kinetic insights into the atmospheric degradation of emerging halogenated OVOCs.

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# Theoretical Design and Electronic-Structure Engineering of Donor–Acceptor π-Conjugated Molecular Systems for Tunable Nonlinear Optical Properties

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**Abstract**

The rational design of molecular materials with tunable optical and electronic properties is of considerable importance for the development of advanced nonlinear optical (NLO), optoelectronic, photonic, and photovoltaic technologies. In the works discussed here, density functional theory (DFT) and time-dependent density functional theory (TD-DFT) have been employed to systematically investigate the structure–property relationships of diverse donor–acceptor molecular and inorganic–organic hybrid systems. The studied systems include difluoroboron–naphthyridine analogues, donor–acceptor functionalized $B_{12}N_{12}$ nanoclusters, BODIPY-based zwitterionic molecules, indole-based donor–π–acceptor dyes, nickel dithiolene derivatives, and cyanide-substituted 5,7,12,14-tetraazapentacene (N4PENT) derivatives. Particular emphasis is placed on understanding how electron-donating/electron-withdrawing substituents, π-conjugated linkers, substitution patterns, and molecular architecture influence frontier molecular orbital energies, HOMO–LUMO gaps, electronic transitions, charge-transfer characteristics and nonlinear optical responses. The theoretical results demonstrate that appropriate donor–acceptor combinations and extension of π-conjugation can effectively regulate electronic delocalization and charge-transfer pathways, leading to significant changes in absorption characteristics, polarizability, and first- and second-order hyperpolarizabilities. Complementary analyses based on frontier molecular orbitals, density of states, molecular electrostatic potential, transition dipole moment density, electron–hole distribution, $\Delta r$ index, ionization potential, electron affinity, and reorganization energies provide molecular-level insight into the origin of the observed optical and charge-transport properties. In particular,

strong donor–acceptor interactions and suitable π-linkers are found to promote enhanced NLO responses. Overall, the combined theoretical investigations highlight donor–acceptor engineering, π-conjugation, and controlled functionalization as powerful strategies for developing molecular materials with tailored nonlinear optical properties.

**Keywords**

Donor–acceptor systems; π-conjugation; density functional theory; nonlinear optical properties; hyperpolarizability; charge transfer; optoelectronic materials; molecular design.

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# Role of excited states in optoelectronics: A model exact and DMRG Study

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Electronic structure calculations and relative energy ordering of singlet and triplet energy eigenvalues play an important role in determining the properties of the organic conjugated molecules in the field of optoelectronics. These molecules are represented within model Hamiltonian and diagonalized exactly for ground and few low-lying excited states in singlet and triplet subspaces for relatively smaller sizes. An approximate Density-Matrix-Renormalization (DMRG) technique is used in calculation in order to manage comparatively bigger system size. This talk also highlights the implementation of a DMRG scheme that can treat a molecular systems with periodic boundary condition (PBC). PBC-DMRG results are in very good agreement with experiments and *abinitio* results for cycloparaphenylene and cyclophenacene molecules.

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**Keywords: Theoretical Model; Electronic Structure; DMRG ; Optoelectronics**

# Insights Into Antibacterial Action of Transition Metal Dichalcogenides

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Two-dimensional transition metal dichalcogenide (2D TMD) nanomaterials, such as $MoS_2$ and $WS_2$, have recently attracted significant attention due to their effective broad-spectrum antibacterial activity, combined with excellent biocompatibility and a low tendency to induce bacterial resistance. Herein, using a series of atomistic molecular dynamics simulations studies, we attempt to provide an in-depth understanding of the underlying mechanism of their antibacterial action against the Escherichia coli (*E. coli*) and Staphylococcus aureus (*S. aureus*) bacterial membranes.[1-3]

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**Keywords:** Antibacterial activity, $MoS_2$, $WS_2$, Nanosheets

# Exciton-Plasmon Coupling in Plasmonic Perovskite Nanocrystals

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Plasmonic materials exhibit strong light absorption properties, leading to their usage in solar energy conversion. In this regard, plasmonic metal/semiconductor hybrid nanomaterials have been extensively studied, however, limited to chalcogenide semiconductor nanocrystals (NCs). While perovskite NCs have been at the forefront of solar energy research over the last few years, the corresponding plasmonic hybrids are largely missing in the literature. We prepared epitaxial Au@CsPbBr3 hybrid plasmonic perovskite nanocubes and nanoplates using a molecular shuttle at the water-hexane interface.[1] The Au@CsPbBr3 NCs exhibit simultaneous exciton resonance and localized surface plasmon resonance (LSPR) with equal dominance, covering the full visible region, allowing a strong exciton and plasmon coupling to form a hybrid quasi particles, called plexcitons. The plexciton formation is further evident from a large Rabi splitting, anti-crossing behavior followed by suppressed exciton scattering, as observed in Ag@CsPbCl3 NCs and Au@CsPbBr3 nanoplates. [2,3] Ultrafast spectroscopy reveals fast charge transfer from CsPbBr3 to Au domain and can be effectively modulated using small molecule probes, such as benzoquinone and pyridine. Further, we show that the monolayer thin Au@CsPbBr3 nanoplates can detect single molecules in as low as sub-atto-molar concentrations using surface enhanced Raman scattering (SERS) technique via simultaneous electromagnetic and plasmon induced charge transfer mediated chemical enhancement. [4]

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**Keywords:** Plasmonic perovskite, plexciton, nanocrystals, ultrafast dynamics

# Reinventing the Drug Formulation Technology for Improved Onset of Action and Lower Dose Requirements

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Active pharmaceutical ingredients (APIs) are the major components of drug molecules in treating the diseases. Currently, about 60-70% of available drugs are reported to have poor aqueous solubility, and this number is expected to increase as the pharmaceutical industry shifts its attention to more complex APIs. The standard practice includes extensive use of excipients to improve the solubility. However, these excipients often cause serious side effects. Here, we reinvent the API formulations by conjugating the APIs with certain biocompatible organic moieties that not only avoid the use of excipients, but also enhanced the solubility of the APIs many folds. Our preliminary results from solvation energy calculations and *in-vitro* measurements on over-the-counter-drugs - aspirin, paracetamol, ibuprofen, diclofenac showed 100 -1000 fold improved solubility of the reformulated-APIs (rAPIs) in comparison to the parent APIs. Dissolution studies showed much faster availability of the rAPIs in solution than the parent APIs, signifying rapid onset of action. *In-vivo* pharmacokinetics and pharmacodynamics studies of the rAPIs in rat model showed significantly higher $C_{max}$ and shorter $T_{max}$ than the APIs or even marketed formulations. Due to their exceptionally high solubility and higher $C_{max}$, rAPIs can be delivered in liquid form with lower dose requirements. Currently, this technology is being implemented to reformulate various life-saving drugs for improved efficacy and cost effectiveness.

Keywords: Drug reformulation; Solubility and Rate of Dissolution; Pharmacokinetics and Pharmacodynamics Studies; Simulations and Experiments.

# Buckling and Defects in Two – Dimensional Atomically Thin Monolayers

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**Keywords**: Two-Dimensional Systems; Phase-transitions; Symmetry breaking in materials

## Abstract

Graphene has emerged as one of the most fascinating areas of research in condensed matter and materials science. Apart from graphene, several other 2D analogues like silicene, phosphorene, MXenes, $MoS_2$, germanene have been recently isolated and characterized. One unifying theme among these new materials is that unlike graphene, they are non-planar. The mode and measure of the buckling (puckering) from planarity depends on the local electronic structure. The effects of such ripples are manifold particularly in its local reactivity to halogens and hydrogens along the more ~$sp^3$ atoms. Pseudo Jahn-Teller (PJT) distortions is shown as a central unifying concept that explains the overall structural preferences of these systems. The extent of buckling also leads to interesting and emerging phenomenon like phase-transitions into Topological Insulators from normal semi-metal due to spin-orbital coupling (SOC). The effect of PJT in bestowing structural diversity and novel electronic and spin phases in 2D-monoatomic layers will be discussed in this lecture.

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# Cavity Ring-down Spectroscopy in Gas and Condensed Phases

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Cavity ringdown spectroscopy (CRDS) has proven to be a highly sensitive technique for *in-situ* measurement of optical extinction and has been widely applied across various media, including gases, liquids, plasmas, and aerosols. Evanescent wave (EW)-CRDS is a powerful technique for probing interfacial extinction dynamics. It has been extensively employed to investigate nanoparticle adsorption kinetics on functionalized silica surfaces, enabling real-time, in situ monitoring of interfacial processes with high sensitivity. In this talk, I will give a glimpse into the high-resolution spectroscopic probing of site-specific $N_2O$-isotopologues in the gas-phase using CRDS [1]. We propose a unique spectral window in the 7.8 µm mid-IR region that is free from spectroscopic interference from major atmospheric constituents, enabling simultaneous high-resolution detection of the two site-specific isotopologues of nitrous oxide, $^{14}N^{15}N^{16}O$ and $^{15}N^{14}N^{16}O$. I will subsequently explain the EW coupled-CRDS probing of Guanidine hydrochloride (GdnHCl)-induced Gold nanoparticles (GNPs) aggregation kinetics in real-time with high sensitivity. Additionally, we explore the influence of L-tryptophan (L-Trp) on this aggregation process, revealing a distinct phenomenon of "frustrated aggregation", where the interplay between guanidinium ions and aromatic amino acids alters the conventional aggregation pathway [2]. The extinction dynamics measured via EW-CRDS provide quantitative access to real-time aggregation kinetics with sub-nanometer sensitivity, establishing the technique as a powerful tool for probing nanoscale colloidal interactions.

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**Keywords:** Cavity ring-down spectroscopy; Evanescent wave; Gold nanoparticles

# Thermophysical and dynamical properties of liquid sodium: Insights from MD simulations and DFT-BTE theory

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Liquid sodium plays a vital role in advanced thermal systems and nuclear reactor applications, necessitating a detailed understanding of its flow and heat transfer behavior in both bulk and confined states. The present talk will explore the behavior of liquid sodium in bulk and under confinement using the tools of molecular dynamics (MD) simulations, density functional theory (DFT) and Boltzmann transport equation (BTE). The thermophysical properties of sodium metal over a wide range of temperature was studied. Density functional theory (DFT) and Boltzmann transport equation (BTE) were used to evaluate the electronic thermal conductivity and MD was used to calculate the phonon thermal conductivity of the sodium metal. Non-equilibrium MD (NEMD) simulations were further performed to investigate flow and heat transfer characteristics of sodium metal under nanoscale confinement. The multiscale findings demonstrate that interfacial effects dominate heat transfer under nanoscale confinement.

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**Keywords:** three to five keywords, separated by semicolons

# Water Dynamics in Biomolecular Condensates: Beyond Slow Biomolecular Diffusion

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Biomolecular condensates provide distinct environments for biochemical processes, yet the dynamics of water within these environments remain poorly understood. Fluorescence recovery after photobleaching (FRAP) measurements have revealed that biomolecular translational diffusion can be slowed by more than three orders of magnitude inside condensates. Does water experience a comparable dynamical slowdown? Here, we directly probe isotopically diluted water using two-dimensional infrared (2D IR) spectroscopy to investigate its local hydrogen-bond dynamics across condensates of varying composition. Complementary NMR measurements quantify the translational diffusion of water, connecting local dynamics with molecular transport. Both measurements reveal only a modest slowdown of water within condensates, in striking contrast to the pronounced retardation reported for biomolecules. These results demonstrate that severely restricted biomolecular mobility can coexist with relatively rapid water dynamics. This disparity highlights the species-dependent nature of condensate dynamics and cautions against using biomolecular diffusion alone to infer the dynamical environment experienced by water. Our findings provide a molecular perspective on condensate interiors and their capacity to support transport and biochemical activity.

**Keywords:** condensates, water, dynamics, 2DIR, diffusion

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

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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 transport[3] . Extending this framework, we reveal that RNA-like polyelectrolytes exhibit a remarkable dual role governed by the underlying interaction landscape. While RNA-like polyelectrolytes destabilize 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 materials[4,5] .

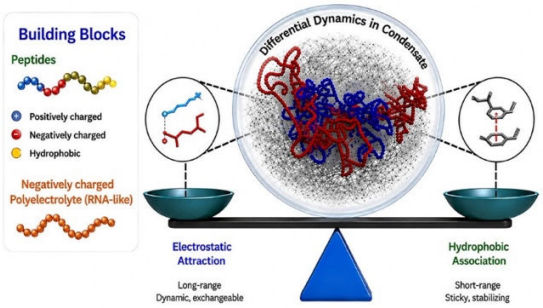



**Figure 1. Dynamics in heterotypic condensates mediated by competition between short and long range interactions**

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**Keywords: Intrinsically Disordered Peptides, Phase Separation, Diffusivity, Liquid-like nature**

# Epitaxial Assembly of 1D/2D Organic Lateral Heterojunctions for Integrated Photonics

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Two-dimensional organic lateral heterostructures (2D OLHs) hold immense promise for integrated optoelectronic and photonic applications. However, achieving precise control over nucleation, crystallographic orientation, and interfacial defects during solution-phase synthesis remains a major challenge. Here, we report the controlled synthesis of high-quality 1D and 2D epitaxial heterojunctions [1,2] constructed from two distinct benzothiadiazole-based organic crystals with red and green luminescence using a sequential solution self-assembly approach. By selectively tuning nucleation kinetics, we achieve spatial architecture control to yield both symmetric green-red-green (G-R-G) and red-green-red (R-G-R) multi-block heterostructures (Figure 1). The resulting 2D OLHs feature lateral dimensions of ~20 μm and a tunable thickness ranging from 20 to 400 nm. Guided by a screw dislocation growth mechanism, the spiral arrangement of molecules within the lattice effectively accommodates volume variations and lattice strain, thereby minimizing interfacial connection defects. Benefiting from high structural integrity and seamless lateral interfaces, these multi-dimensional organic heterostructures demonstrate efficient optical waveguiding and spatially tunable exciton conversion, offering a robust strategy for integrated organic photonic systems.

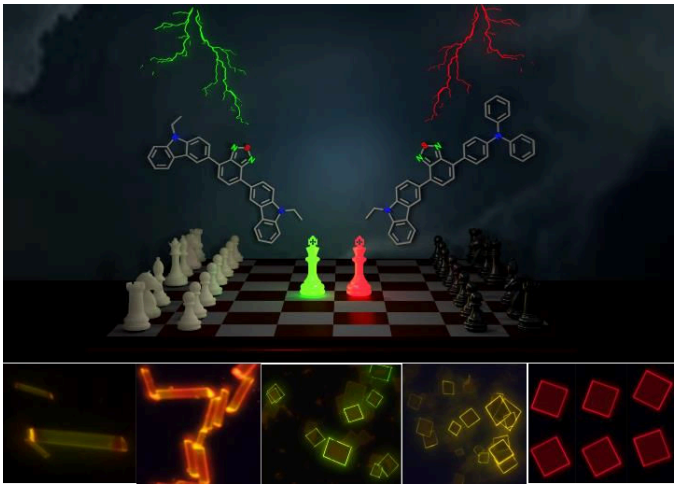


**Figure 1.** The two molecules that grow together epitaxially and emit with different colours on excitation.

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**Keywords:** epitaxial assembly; organic crystals; 1D/2D lateral heterojunctions; integrated photonics

# Transient collective motion and density voids in a model drying chemotactic bacterial film

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We present a two-dimensional active-hydrodynamic theoretical model of run-and-tumble *Escherichia coli* drying in its own broth around a central sugar source. The framework combines outward capillary transport, chemotactic bias, active-Brinkman hydrodynamics, and a peripheral-to-inward rheological-arrest front. The mobility-arrest law is constrained by the measured broth complex viscosity at $25^{\circ}C$, and the temperature dependence of the broth rheology is used to predict the temperature dependence of the collective-motion window with no additional adjustable parameters.

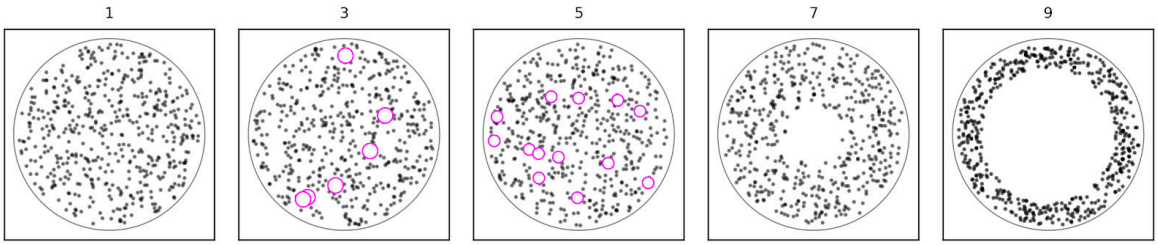



**Figure 1.**Experimental drying sequence at $25^{\circ}C$.

**Keywords:** collective behavior of motile cells; Low-Reynolds-number motions; Suspensions

# Engineering Chemical Reactivity and Optical Response through Defect Design in Nanocluster Assemblies

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Defects and dopants are often regarded as perturbations of nanoscale materials; however, their deliberate incorporation offers an opportunity to create new chemical environments and emergent functionality. Our work explores how metal-ion incorporation can be used to program the structural, electronic, photophysical, and chemical properties of atomically assembled nanoclusters. Using zinc-mediated gold nanocluster assemblies as a versatile platform, we demonstrate that the identity and local environment of incorporated metal ions can profoundly reshape molecular interactions and optical behavior. Lanthanide incorporation, exemplified by $Eu^{3+}$, induces local structural distortion, electronic-state localization, and symmetry-dependent emission while simultaneously generating chemically addressable Lewis-acidic sites for molecular recognition.[1] More importantly, $Mn^{2+}$-derived defect states are shown to fundamentally alter the chemical reactivity of the assemblies: uric acid interacts with defect-containing and defect-free assemblies through distinct pathways, leading to opposite fluorescence responses and enabling ratiometric optical reporting.[2] Complementing these defect-engineering strategies, we develop metal-mediated nanocluster assemblies in which selective thiol coordination produces a robust dual-emission response suitable for operation in complex biological media.[3] Collectively, these studies establish a broader framework in which nanoscale defects and dopants are transformed from structural perturbations into programmable chemical sites, allowing molecular recognition, coordination chemistry, and excited-state processes to be coupled with optical readout. This approach provides a foundation for designing multifunctional nanomaterials in which chemical reactivity and photophysical function can be rationally programmed for molecular interrogation and biological diagnostics.

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**Keywords:** Defect engineering; nanocluster assemblies; molecular recognition; coordination chemistry; optical reporting

# A Bayesian Lens on Molecular Rigidity: Learning Atomic Weights from Ensemble Data

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The standard measure of comparing structures in molecular dynamics (MD) simulations is the root-mean-square deviation (RMSD). RMSD weighs every atom equally. Hence a few highly mobile domains, such as loops or disordered regions of a protein, can dominate the quantity, while the rigid, functionally important core has marginal contribution. Typical work around involves manual exclusion of mobile atoms. However, that depends on prior knowledge of the system and is hard to apply consistently across systems. We present a Bayesian alternative, Bayes-optimal RMSD (BRMSD), that learns per-atom weights directly from the ensemble data. Structure and weights are optimized together by minimizing a single free energy that balances low deviation against a penalty for straying from uniform weighting. The same free energy, adapted with different bias terms, yields five related analyses: global alignment, focused alignment, trajectory smoothing, soft clustering of conformational states, and rigid-domain identification. All of these modules are implemented in the open-source Python package `BRMSD`. BRMSD is benchmarked on a membrane protein (endoplasmic reticulum associated translocon protein SND3) and a phosphotransferase (adenylate kinase, ADK). BRMSD automatically concentrated weight on each system's rigid core, lowering the apparent RMSD threefold without manual atom selection. Moreover, it correctly separated ADK's open and closed conformational states and recovered its three known rigid domains in the correct order of rigidity. BRMSD offers a reproducible way to compare, cluster, and decompose molecular structures, applicable to any system studied by MD, from folded proteins to nucleic acids and disordered ensembles.

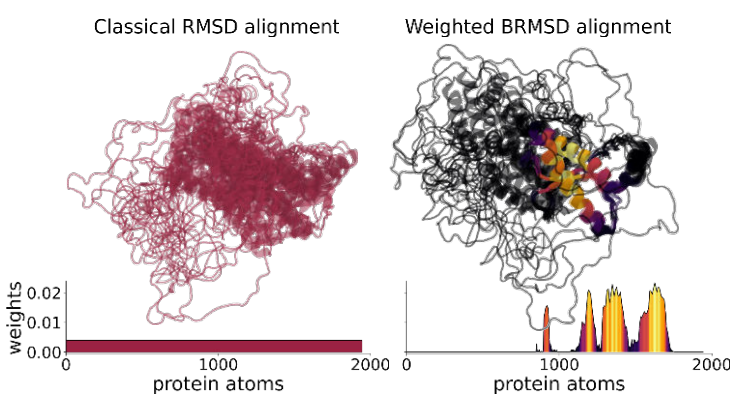



**Figure 1.** Ensemble alignment of a protein with intrinsically disordered regions using classical RMSD (left) and BRMSD (right). The graphs show the atomic weights. Rigid regions receive more weights in BRMSD.

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**Keywords:** Alignment; RMSD; Bayesian inference; MD simulations

# Small-Molecule-Directed Self-Assembly of Amino Acids for Emergent Fluorescence

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Engineering fluorescence from natural biomolecules without covalent modification offers a sustainable approach to functional optical materials. However, the molecular principles governing the emergence and tunability of fluorescence during biomolecular self-assembly remain poorly understood. In this talk, I will discuss how small-molecule-directed self-assembly can transform the intrinsic photophysics of amino acids through distinct molecular- and solvent-mediated mechanisms. Phenylalanine (Phe), a weakly fluorescent amino acid, exhibits a remarkable enhancement in emission upon hydrazine (Hyd)-mediated self-assembly, accompanied by a shift in the emission maximum from 290 nm ($\lambda_{ex}$ = 240 nm) to 490 nm ($\lambda_{ex}$ = 410 nm) [1]. The quantum yield increases nearly tenfold, from 0.2% for monomeric Phe to 20.7% for the assembly. FE-SEM reveals well-defined stacked sheet-like architectures rather than conventional fibrillar structures, suggesting an ordered organization mediated by π–π stacking and hydrogen bonding. The assemblies further form fluorescent, hygroscopic hydrogels, highlighting their potential for moisture management and biomedical applications [1].

A complementary strategy using tryptophan (Trp) reveals distinct morphologies and photophysical properties depending on the small molecule directing the assembly. Co-assembly with L-ascorbic acid (Asc, pH ~3) suppresses native Trp emission and generates a broad band at 470 nm ($\lambda_{ex}$ = 380 nm), corresponding to a 120 nm red shift. In contrast, hydrazine (Hyd, pH 10) accelerates assembly by ~2.5-fold and produces larger spherical assemblies with emission at 430 nm ($\lambda_{ex}$ = 345 nm) [2]. Molecular dynamics and metadynamics simulations reveal fundamentally different roles of these small molecules: Asc directly associates with Trp, whereas Hyd primarily reorganizes the hydration environment and reshapes the Trp–Trp association landscape. Together, these findings demonstrate that molecular recognition, solvation, and intermolecular organization can be independently modulated to engineer emergent fluorescence from native biomolecules, providing a versatile noncovalent strategy for developing sustainable supramolecular fluorophores.

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**Keywords:** self-assembly, amino acids, fluorescence

# Quantum Nuclear Dynamics: Reactive Scattering and Vibronic Coupling

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We present time-independent and time-dependent quantum studies of reactive scattering and of vibronic coupling, all performed on accurate ab initio PESs.

For O + $O_2$ isotope exchange, time-independent calculations on the ozone PES reveal an insertion mechanism at low collision energy, with forward–backward symmetric differential cross sections, giving way to direct abstraction at higher energy [1]. For N + $N_2$ exchange on the ground $^4A''$ PES, time-dependent wave packet (TDWP) and quasiclassical trajectory (QCT) calculations for $^{15}N + {}^{14}N_2$ and $^{14}N + {}^{15}N_2$ show a double barrier enclosing a shallow well, which traps a short-lived complex and imprints plateaus on the reaction probability [2,3]. Including Coriolis coupling (CC) lowers the thresholds that the centrifugal-sudden approximation overestimates at high total angular momentum. Vibrational excitation lowers the threshold but suppresses reactivity at high energy, as translational energy becomes more effective than vibration [2,3]. The barrierless S + SD reaction proceeds mainly by abstraction through a long-lived complex; at vibrational level $v = 10$ the mechanism turns direct, and a QCT/QM-$\alpha J$ extrapolation reproduces quantum cross sections at a fraction of the cost [4].

Turning to spectroscopy, a 5 × 5 diabatic vibronic Hamiltonian for the five lowest electronic states of the aromatic $P_2N_3$ radical, containing multiple conical intersections, reproduces the 193 nm photoelectron spectrum of $P_2N_3^-$: the first band arises from four coupled states and the second from the $\tilde{D}$ state, with electronic population transfer within about 50 fs [5].

Together, these studies show that quantum effects, namely Coriolis coupling, resonances and nonadiabatic coupling, become decisive as rotational, vibrational or electronic excitation increases, offering a common framework for isotopic, vibrational and electronic phenomena in atmospheric, interstellar and cluster chemistry.

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**Keywords:** reactive scattering; wave packet dynamics; vibronic coupling; conical intersections; isotope effects

# A systematic Green's function formalism for kinetic energy density

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The density functional theory, in principle, bypasses the need for a many-electron, Fermionic, ground state wave function for describing electronic structures of atoms and molecules. In Kohn-Sham scheme [1], one needs to solve a set of coupled integro-differential equations leading to polynomially increasing computational cost with the increase in number of electrons. Orbital-free density functional theory(OFDFT), on the other hand, requires only one Euler-Lagrange equation to get the true ground state electron density[2, 3]. The lack of an adequately approximated kinetic energy density functional remains the bottleneck to achieve this goal in practice. In recent years, however, there is a resurgence in this area of research[4, 5]. In this talk, we will discuss the possibilities and challenges to develop a functional approach with OFDFT drawing upon our recent works. In these works [6–8], Green's function approach have been devised to come up with a practical and systematic scheme to compute the kinetic energy without recourse to any model. The resultant formalism solves the problem of systematic development of kinetic density functionals that plagues the density functional theoretical approximations. Moreover, this methodology can be applied to systems with arbitrary spin multiplicities. We will discuss the methodology and its promising results provided by the flagship applications.

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# From Descriptors to Discovery: A Physics-Informed Inverse Design Framework for Self-Trapped Excitons in Unexplored Halide Perovskites

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Self-trapped excitons (STEs) underpin broadband luminescence in perovskites, yet the microscopic rules governing their formation — and strategies for discovering new STE-active materials — remain poorly established. We present a unified framework spanning first-principles physics to data-driven inverse design, targeting unexplored halide perovskite chemistries. In the first part, we systematically investigate STE formation across oxide, halide, and hydride perovskites by combining lattice-dynamical analysis, mode-resolved electron-phonon coupling calculations, and constrained ΔSCF excited-state relaxations. We demonstrate that STE stabilization is governed by the cooperative interplay among electron-phonon coupling strength, vibronic reorganization, and structural distortion — quantities unified into a physics-inspired composite descriptor that delineates a phase diagram of delocalized, intermediate, and strongly self-trapped excitonic regimes across chemically diverse perovskite families. In the second part, we leverage these physically motivated descriptors within a machine-learning inverse-design framework to predict unconventional double- and triple-halide perovskites that have not yet been experimentally explored. By targeting specific electronic properties — including band edge characteristics and excitonic response — the framework proposes candidate materials with tailored STE behavior, effectively inverting the structure-property relationship established in the first part. Together, this physics-to-prediction approach transforms the analysis of exciton localization from system-specific case studies into a transferable, descriptor-driven strategy for accelerated luminescent materials discovery.

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**Keywords:** Self-trapped excitons; electron-phonon coupling; perovskites; descriptor-based phase diagram; inverse design

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# Ultrafast Mapping of Nonradiative and Radiative Pathways in Dual-Conformer TADF Emitters

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Organic light-emitting diodes based on thermally activated delayed fluorescence (TADF) can achieve near-unity internal quantum efficiency by thermally upconverting non-emissive triplet states to emissive singlets without heavy metals [1]. In donor-acceptor (D–A) TADF emitters, a small $\Delta E_{ST}$ and the favourable energetic ordering of the $^1$CT, $^3$CT, and $^3$LE states can facilitate reverse intersystem crossing (rISC) and TADF [2]. However, how conformational dynamics govern access to these states in flexible systems such as PTZ-TRZ, where quasi-axial (QA) and quasi-equatorial (QE) conformers coexist with a small energy separation [3], remains unclear. Their populations and interconversion are influenced by donor substitution and solvent polarity [4,5], generating distinct relaxation pathways that compete with TADF. Here, we investigated three D-A -type emitters with varying degrees of conformational rigidity that exhibit dual emission from coexisting QA/QE conformers. Excitation-dependent femtosecond transient absorption spectroscopy (fs-TAS), combined with time-resolved emission spectroscopy, is used to probe dark and emissive states and identify competing pathways [6]. We demonstrate that QA↔QE interconversion plays a critical step in governing TADF. Excitation induces LE→CT conversion in QA, which predominantly follows a TADF-inactive pathway, whereas its conversion to QE redirects the population into a resonantly aligned manifold that enables efficient rISC. Our results demonstrate that both molecular structure and solvent polarity regulate the conformational equilibrium, thereby controlling the balance between radiative and nonradiative relaxation and ultimately determining TADF activity. These findings establish design principles for TADF emitters by controlling conformational dynamics, excited-state energetics, and environmental polarity.

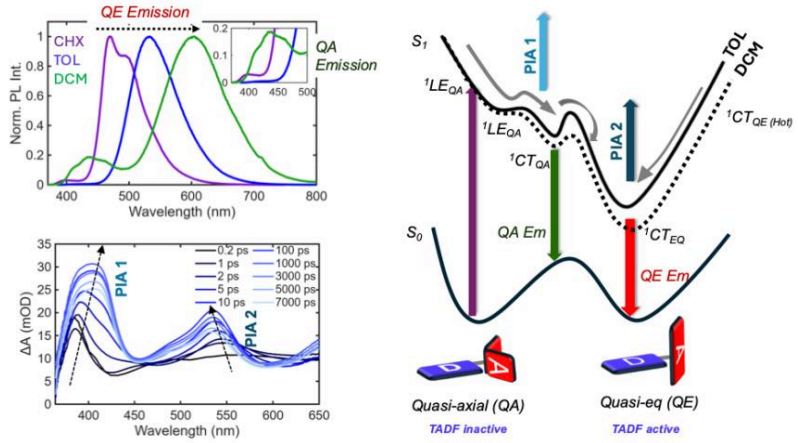



**Figure 1:** Schematic illustration of quasi-axial and quasi-equatorial conformers, fs-TAS spectral traces and conformer-dependent excited-state evolution and relaxation pathways in D-A TAF emitters.

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**Keywords:** Thermally activated delayed fluorescence; Femtosecond transient absorption; Confirmation dynamics, Excited state relaxation

**Arijit Kumar De**
IISER Mohali

Also presented as invited poster **IP-17** (Poster Session B)



# Unveiling Time-Dependent Vibronic Coupling by Third- and Fifth-order Raman Spectroscopy

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In this presentation, I will give an overview of the research being pursued in our group, with a particular emphasis on why one should go beyond pump-probe spectroscopy, highlighting the need for advanced methods like impulsive stimulated Raman spectroscopy (ISRS) in the context of a classic problem (i.e., polar solvation dynamics). Then, with the specific example of the coupling of charge carriers with lattice vibrations in lead-free double-perovskite nanocrystals, I will discuss how one can estimate electronic-state-specific carrier-phonon coupling and can monitor the time evolution of coherent vibrational dynamics in real time via a two-pulse (Raman pump/probe) third-order ($\chi^3$) measurement using wavelet analysis. I will also discuss how this method can be further extended to a fifth-order ($\chi^5$) measurement to investigate phonon dynamics over a longer timescale.

**Keywords:** Impulsive stimulated Raman scattering, vibronic coupling, charge-carrier/phonon coupling.

# Hydrophobic Amino Acid Solutions at Work: Do They Reshape Protein Solvation and Thermal Stability?

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Protein instability remains a major challenge during the manufacturing, transportation, and storage of therapeutic proteins. Although liquid protein formulations are widely preferred for their clinical convenience and relatively low production costs, proteins in solution can undergo aggregation, unfolding, and other forms of degradation during storage. The use of excipients, particularly amino acids, is an established strategy for improving protein stability in liquid formulations. [1]

Unlike highly polar amino acids, hydrophobic amino acids can preferentially associate with exposed nonpolar patches on proteins and alter conformational stability. In this talk, I shall emphasize the molecular basis of protein thermal stabilization using extensive all-atom molecular dynamics simulations of ubiquitin in pure water and in the aqueous solutions of the hydrophobic amino acids alanine, valine, isoleucine, and phenylalanine at two different temperatures. [2] We observed that the different hydrophobic amino acids stabilize ubiquitin through distinct molecular mechanisms. While alanine exhibits the strongest and most homogeneous association with the protein surface, facilitated by its small side chain and efficient surface packing, valine and isoleucine provide intermediate stabilization, where hydrophobic interactions are balanced by steric effects that restrict surface accessibility. Phenylalanine, despite weaker direct protein interactions due to its bulky aromatic side chain and propensity for aggregation, promotes stabilization through a more indirect mechanism involving a structured, persistent hydration environment. The discussion will further elucidate protein thermal stability by coupling changes in solvation structure, solvent dynamics, and hydrogen-bonding networks, with the underlying stabilization mechanism strongly dependent on amino acid side-chain size, surface accessibility, and propensity for aggregation.

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**Keywords:** hydrophobic amino acid solution; solvation; protein stability; simulation; thermal unfolding

# Specific DNA Recognition Induces Folding Transition of the Oncogenic Fusion Protein PAX3FOXO1

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Alveolar Rhabdomyosarcoma (aRMS), an aggressive subtype of one of the most common paediatric cancers, has been characterized by the presence of primarily two fusion proteins: PAX3FOXO1 and PAX7FOXO1[1] . PAX3FOXO1 (P3F) shows aberrant transcriptional behaviour by upregulating the PAX3 target genes[2]. However, the underlying molecular mechanism, more specifically, how DNA recognition through its DNA binding domain (DBD) drives conformational reorganization of the distant FOXO1-derived regulatory low complexity domain (LCD) yet remains poorly understood. We here employ µs–scale atomistic molecular dynamics simulation, and reveal that upon DNA binding, P3F adopt similar size but its exposure to solvent increases. The DBD gets more stabilized while significantly affecting the dynamics of distal LCD. These changes are associated to redistribution of intra- to inter-molecular non-bonded interactions, including hydrogen bonds, salt bridges, and cation-pi interactions. Most importantly, the effects have impacted beyond the DNA interacting residues from DBD, indicating long-range communication between the DNA and transcriptional regulatory regions of P3F. Our study provides a molecular framework for understanding of how DNA recognition can reshape the structural and dynamic landscape of P3F, potentially contributing to its aberrant transcriptional activity in ARMS.

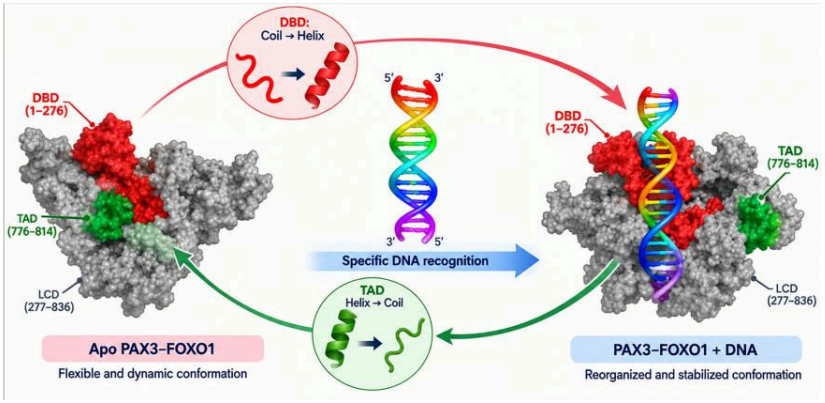



**Figure 1.** Schematic representation of DNA-induced conformational remodeling of PAX3–FOXO1

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**Keywords:** Alveolar Rhabdomyosarcoma, Fusion Protein, DNA-Binding Domain (DBD), Low-Complexity Domain (LCD), Transcriptional Regulation.

# Reset controlled Non-equilibrium Transition in an Inhomogeneous Brownian Information Engine

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We investigate a Brownian information engine (BIE) driven by space-dependent diffusivity $D(x) = D_0(1\pm x^2)$. The working protocol is described by overdamped Langevin dynamics within a harmonic confinement and is controlled via resetting. The geometry of the space-dependent diffusivity significantly impacts information processing. If the fluctuations increase while moving away from the potential's center $D(x) = D_0(1 + x^2)$, a higher information-energy exchangeability is observed. This colossal information processing is hindered by a lower resetting cycle time. Interestingly, a case of space-dependent fluctuations, whose strength vanishes as one moves away from the potential center $D(x) = D_0(1 - x^2)$, enables reset-controlled thermodynamic phase behavior. In the slow-resetting limit ($r \to 0$, the system exhibits an athermal engine-refrigerator transition governed by the ratio between the frequency of confinement and the space-dependent fluctuation $\alpha = k/2D_0$ . The engine can convert the acquired information into positive work only if $\alpha > 1$ reveals a noise-induced thermodynamic phase transition. Moreover, a finite cycle time acts as a non-equilibrium control field, redistributing the probability by shifting the engine-refrigerator phase boundary. Our analytical predictions are supported by Langevin simulations and contrasted with the homogeneous diffusivity, highlighting the distinct role of multiplicative noise in enabling reset-controlled information use.

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**Keywords:** Brownian information engine, Space-dependent diffusivity, Reset-induced transition, Stochastic thermodynamics

# Stochastic Resetting Prevails Over Sharp Restart for Broad Target Distributions

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

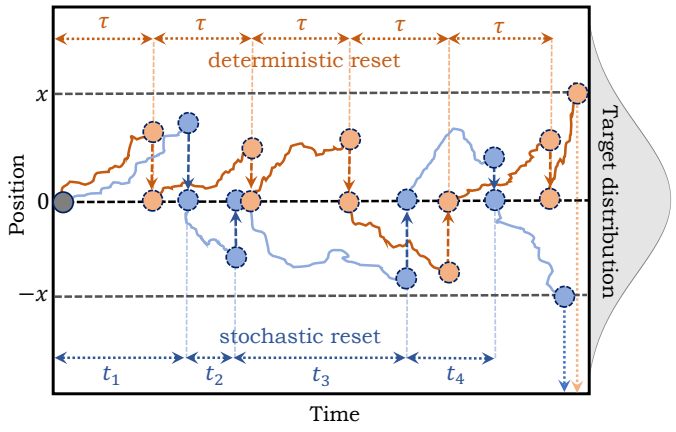



**Figure 1**: *A schematic position vs time diagram for diffusion with resetting (in 1D), where an absorbing target is located at a random distance chosen from a distribution of target centered around the origin (in gray).*

## References

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**Keywords:** Stochastic resetting, diffusive system, mean first-passage time, waiting time distribution.

# Role of Photoinduced Processes to Modulate the Optical Properties of Carbon Nanoparticles

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**Abstract:** Modulation of optical properties of carbon nanoparticles in solution is still a debatable area of ongoing research on graphene oxide (GO) based nanoparticles and carbon quantum dots. Proper understanding of the photophysical processes dependent upon the presence of different surface functional groups, nature of the additives like polymers, surfactants and metal ions may open up the promising applications of these nanoparticles for their minimal in vivo and in vitro toxicity. We have investigated the possible origin of modulation of the optical properties by using steady state and time resolved fluorescence spectroscopic techniques. The findings of the study will aid further research on the photoluminescence characteristics of the various members of the family of carbon nanoparticles. Unveiling of the structural heterogeneity and the insights to the role of different photoinduced processes in these nano systems are valuable for multidimensional applications which include optoelectronics, energy storage, biological fields, and the development of optical nano sensors for detecting environmentally hazardous substances and biologically important molecules.

**Bio sketch:** Prof. Arnab Halder is the head of the Department of Chemistry at Presidency University, Kolkata, India. He was awarded his Ph.D. from the Indian Association for the Cultivation of Science, Jadavpur, India. He served as a Visiting Researcher at the Molecular Photoscience Research Center, Kobe University, Japan, focusing on Coherent Control by Pulse Shaping Technique. He has expertise in Ultrafast Spectroscopy for studying various photophysical processes and is currently working on the synthesis and spectroscopic characterization of carbon nanomaterials and their applications in biology and environmental science.

# Probing cancer biomarkers using a biophysical approach

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We explored cancer cell-derived extracellular vesicles (EVs) and metaphase chromosomes to probe cancer biomarkers. EVs are naturally occurring lipid bilayer-enclosed nanoparticles involved in intercellular communication [1]. Hyaluronan (HA), a potential cancer biomarker, is a non-sulfated glycosaminoglycan. Our experiments revealed that cancer EVs exhibited significantly higher HA surface densities than normal EVs [2]. We measured the contour lengths of single HA molecules on a cancer EV surface and assessed their mechanical properties [3]. We also elucidated the electrical properties of single-cancer HA-EVs [4]. These strategies could be realized as non-invasive cancer diagnostics in the future. Chromosomes are DNA-histone complexes essential for the inheritance of genetic information to the offspring, and any defect in them is linked to mitotic errors, cancer growth, and cellular aging. Chromosomal instability is a hallmark of many cancers. We addressed how the epigenetic modifier valproic acid affects chromosomal elasticity and electron transport in cancer chromosomes. Using the physical properties of chromosomes, our multiparametric strategy offers a new scope for studying epigenetic dysregulations linked to cancer [5,6].

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**Keywords:** extracellular vesicles; hyaluronan; metaphase chromosomes; atomic force microscopy; cancer biomarkers

# An Efficient Variational Approach for Thermal Density Matrices with Quantum Anharmonic Effects

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Accurate treatment of anharmonic quantum effects at finite temperatures is essential for reliable prediction of molecular thermodynamic properties. Here, we present a McLachlan-type variational approach based on the Bloch equation to efficiently calculate thermal density matrices and vibrational partition functions. The method uses an independent-particle Effective Harmonic Oscillator (EHO) representation, optimizing multidimensional Gaussian wave functions with only two variational parameters: centroids and widths. The resulting Bloch equation-based thermal EHO ($T_B$-EHO) method minimizes the trace of the squared deviation between the derivatives of the exact and model density matrices. This method is assessed for molecular systems over a broad temperature range of 0–1000 K and benchmarked against thermal vibrational configuration interaction (T-VCI) and thermal vibrational self-consistent field ($T_B$-VSCF) calculations. $T_B$-EHO accurately reproduces the reference thermal properties and provides equilibrium constants in good agreement with both $T_B$-VSCF and experimental results. Most importantly, it achieves approximately 98% reduction in CPU time relative to $T_B$-VSCF. These results demonstrate that $T_B$-EHO provides an accurate and computationally efficient framework for incorporating anharmonic quantum effects into the thermal properties of molecular systems, with promising potential for larger and more complex molecules.

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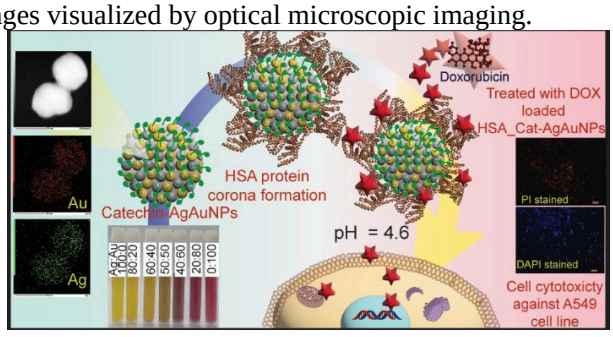
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**Keywords:** Anharmonic quantum effects; Thermal density matrices; Variational theory; Effective harmonic oscillator

# Protein Corona Modulated Doxorubicin Loading and Release from Catechin-Functionalized Ag–Au Alloy Nanoparticles

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A protein corona formed on the surface of engineered nanostructures alters their biological identity as they are introduced to body fluids [1,2]. In this paper [3], we engineered naturally occurring polyphenol, catechin-capped bimetallic Ag–Au nanoparticles as well as their respective monometallic forms and investigated the formation of protein corona taking human serum albumin (HSA) as a model carrier protein (scheme 1). The comparative nature of binding, affinity of HSA toward the catechin-capped bimetallic and monometallic silver and gold nanoparticles, was analyzed with a number of photophysical experiments. Isothermal titration calorimetry and steady state fluorescence analysis revealed the higher binding efficacy of HSA towards bimetallic AgAuNPs than the monometallic Cat-AuNPs and Cat-AgNPs. The formation of the protein corona of HSA on these polyphenol-capped NPs dramatically enhanced the drug loading capacity. The HSA-coronated bimetallic AgAuNPs showed the highest loading percentage of doxorubicin (DOX) (94.64 ± 1.47%) and thereby a higher release percentage (84.37%) at pH 4.6 than that with monometallic Cat-AuNPs and Cat-AgNPs. The release kinetic analysis of doxorubicin from the HSA-coronated Cat-AgAuNPs system supported the non-Fickian diffusion mechanism, i.e., drug release via swelling, erosion, or degradation of the carrier system. The DOX-loaded HSA-coronated catechin-capped NPs showed enhanced cell cytotoxicity against the A549 lung cancer cell line, among which Cat-AgAuNPs showed the highest reduction in cell viability as revealed by the MTT assay and the cytomorphological changes visualized by optical microscopic imaging.




**Scheme 1:** Summary of the work [3].

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**Keywords:** Protein Corona; Bimetallic Ag-Au alloy NPs; Human serum albumin; Drug delivery; Doxorubicin; Cell cytotoxicity.

# Learning what to trust: A Bayesian framework for protein model refinement

**Samiran Sen**[1,*], Samuel Hoff[2], Tatiana Morozova[1], Vincent Schnapka[1], Massimiliano Bonomi[1]

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Protein structure prediction from sequence has dramatically improved in both accuracy and efficiency in recent years, sparking renewed interest in applying artificial intelligence (AI) approaches to structural biology. However, relying solely on AI predictions is known to be problematic due to structural hallucinations. This raises a fundamental question -- how can we determine what to trust?

In this talk, I will discuss a Bayesian framework developed in our group that provides a powerful way to integrate AI predictions, physics-based simulations, and experimental evidence. I will first introduce **bAIes**, a Bayesian approach that fuses the strengths of AI with molecular dynamics (MD) simulations and illustrates its application to small-molecule docking[1] by sampling relevant ligand-binding pocket conformations. In large virtual screening campaigns involving 50000 small molecules, bAIes shows improved discrimination between binders and non-binders compared to models refined with MD (pROC higher by 26.8%). I will then show how the same Bayesian principle can incorporate cryo-electron microscopy (cryo-EM) and tomography (cryo-ET) data. Here, AI-derived structural information and MD simulations are combined with experimental density maps even when only coarse data are available, recovering high-resolution structural details from it. Together, these two studies underscore how Bayesian frameworks can unify AI, physics, and experiment, providing a principled and trustworthy route toward more accurate and efficient modeling of biomolecular structure and dynamics. [2]

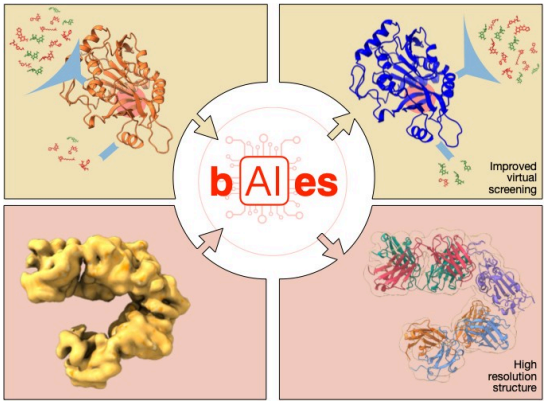



**Figure 1.** Overview of bAIes – a Bayesian inference framework to integrate physics-based force fields with AI-predicted structural confidences to refine protein models.

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**Keywords:** integrative; Bayesian; structural; protein; computation

# Density Functional Theory Study of Single-Atom Catalysts on Porphyrin-like Porous Fullerene for Energy Applications

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Most efficient catalysts for energy harvesting, conversion, and storage often contain rare metal elements.The price of such heavy metals is constantly increasing due to their low natural abundance. This motivates the development of single atom catalysts (SACs), which are hybrid materials containing single atomic sites homogeneously dispersed in a matrix. In SACs every single metal atom is fully available for the reaction, reducing not only the requirement of metal resources, but also the environmental burden after the end of the catalyst life.Therefore, catalytic reactions using SACs are reported to be more economical and environment friendly. In recent days SACs are increasingly employed as electrode components in electrocatalytic and electrochemistry storage applications to enhance the redox kinetics and thereby boosting the efficiencies. Another attractive area in the field is the development of efficient catalyst with the replacement of rare and precious metals by earth-abundant ones. Present study discusses about the catalytic activity of transition metal decorated porous carbon nitride fullerene (M-$C_{24}N_{24}$, M = Fe, Co, and Ni) towards oxygen reduction reaction (ORR) based on density functional theory investigation. It is observed that ORR on these three systems proceeds through more efficient four electron reduction path. The present study reveals that among the three systems, the $O_2$ adsorption energy on the Co-$C_{24}N_{24}$ is in the desirable range to prevent desorption and to sufficiently activate the $O_2$ molecule to proceed through ORR steps at a significant rate. The free energy profiles for the ORR reaction indicate that, all the steps on Co-$C_{24}N_{24}$ are downhill even at increased electrode potential of U= 0.4 V. Thus, the present theoretical study predicts Co-$C_{24}N_{24}$ as better catalyst for the ORR in comparison to Ni-$C_{24}N_{24}$ and Fe-$C_{24}N_{24}$ systems.

**Computational Details:** Spin polarized DFT calculations have been carried out using PAW based electronic structure code, viz. the Vienna ab initio simulation package.

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**Keywords:** ORR, $C_{24}N_{24}$, DFT, SAC

# Molecular Structure and Ultrafast Charge-Transfer Dynamics at Functional Material Interfaces: Insights from VSFG and Transient Absorption Spectroscopy

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In the first part, we present recent advances in nonlinear spectro-electrochemistry, combining surface-specific vibrational sum-frequency generation (VSFG) spectroscopy with electrochemical control to directly monitor charge-transfer processes at solid–liquid and solid–solid interfaces. We discuss how this approach enables in situ molecular-level characterization of the buried interfaces of Prussian blue analogs (PBAs). In the second part, we extend these investigations to ultrafast timescales using transient absorption spectroscopy to probe charge-transfer dynamics at the PBA/ZnO and lead-free $CsSnI_3$ NCs. Overall, our goal is to demonstrate the complementary capabilities of surface-specific vibrational spectroscopy and ultrafast optical spectroscopy for establishing molecular-level structure–dynamics relationships at functional material interfaces.

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**Keywords:** Transient absorption spectroscopy, VSFG, liquid-solid and solid-solid interface

# Proteins in Deep Eutectic Solvents: Molecular Insights from Simulations

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Over the last few years, naturally occurring aqueous deep eutectic solvents (NADES) have garnered significant interest in biophysics, enzyme-catalyzed reactions, and biomolecular engineering. The distinct hydrogen bond network, tunable polarity, and low volatility of NADES provide new avenues for protein stability and functionality that go beyond the capabilities of aqueous solutions. In this presentation, I will discuss our molecular simulation study [1-2] aimed at understanding the atomic-level impact of NADES on protein structure. We investigate the effect of solvent composition and the balance of hydrogen bond donor/acceptor properties on the protein solvation shell using extensive molecular simulations. Key observables such as radius of gyration, RMSD/RMSF, solvent accessible surface area, and secondary structure content reveal how NADES alter protein compactness, flexibility, and stability. The simulations also highlight the role of preferential solvation. These findings provide mechanistic insight into experimentally observed stabilization or destabilization trends in NADES environments.

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**Keywords:** Deep eutectic solvents, Protein solvent interactions, Protein structure

# Domain-Specific Dynamics and Solvent-Controlled Excited-State Proton Transfer in Deep Eutectic Solvents

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Deep eutectic solvents (DESs) show complex microscopic organization and heterogeneity that can strongly affect solvation and chemical reactivity. We present here a combined spectroscopic study of the structural dynamics and photochemical dynamics in two classes of DESs. Steady-state and time-resolved fluorescence measurements using dipolar solutes combined with molecular dynamics simulations reveal the formation of distinct polar and nonpolar domains in amphiphile-based DESs prepared from alkyltrimethylammonium bromides ($C_n$TAB; n = 10, 12, 14) and hexafluoroisopropanol (HFIP). The hydrophobic C153 prefers to reside in the alkyl-chain-rich nonpolar domains, while the hydrophilic C343 localizes in the HFIP- and headgroup-rich polar domains, resulting in significantly different solvation and rotational dynamics[1]. Moreover, these dynamics display strong dynamic heterogeneity, as reflected in their fractional dependence on viscosity and supported by the simulation results. In betaine-based DESs containing ethylene glycol, 1,2-propanediol, or glycerol, the photoacid HPTS exhibits efficient excited-state proton transfer (ESPT), with proton-transfer times on the order of 0.17 to 0.63 ns. Importantly, variation of the hydrogen-bond donor systematically modulates the proton-transfer kinetics through changes in hydrogen-bonding interactions, steric effects, and the local dynamic environment. Solvent relaxation occurs on similar time scales, and both processes are accelerated with increasing temperature, suggesting a strong correlation between proton transfer and solvent reorganization[2]. Together, these results establish nanoscale organization and local solvent dynamics as key determinants of photochemical reactivity in DESs, providing molecular-level aspects for designing task-specific solvent environments.

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**Keywords:** Deep eutectic solvents; Microheterogeneity; Excited-state proton transfer; Fluorescence; Molecular dynamics simulation

# From Interactions to Architecture: Rational Design of Biomolecular Condensate Morphologies

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Understanding how local interactions drive collective organization in many-body systems provides a foundation for the rational design of materials with tailored properties and functionalities. In this talk, I will present our recent efforts to link microscopic interactions to emergent mesoscale organization in protein condensates. I will primarily focus on protein self-assembly through the lens of liquid-liquid phase separation, a key mechanism underlying the formation of biomolecular condensates in cells. I will discuss minimal statistical mechanical models that explicitly incorporate protein internal conformational states and their state-dependent interactions. These models allow us to probe the role of conformationally regulated interactions in selecting condensate morphologies under both equilibrium and non-equilibrium conditions. I will further discuss our recent work based on statistical field theory, which examines how the interplay between quenched disorder and non-thermal noise—features motivated by the intracellular environment—influences condensate morphology and phase behavior. Overall, this talk will illustrate a unified framework based on the modulation of local interactions for the rational design of complex self-assembled architectures of biopolymers.

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**Keywords:** Self-assembly; Phase Diagram; Liquid-Liquid Phase Separation; Biomolecular Condensates

# Engineered Nanoarchitectures for Enhanced Energy Transfer and Multifunctional Applications

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Quantum dot complexes (QDCs), plasmonic-fluorescent nanocomposites (PFNs), and hybrid nanostructures constitute promising functional platforms for manipulating interfacial energy transfer, charge-transfer processes, and photoluminescence for optoelectronic, sensing, environmental, and biomedical applications. This work investigates molecular and interfacial engineering strategies for controlling nanoscale photophysical processes through synergistic coupling of fluorescent metal complexes, quantum dots (QDs), surfactants, and plasmonic nanoparticles. In zinc quinolate complex (ZQC)-Rhodamine B assemblies, surfactant-mediated interfacial organization and QD incorporation regulate donor–acceptor separation, suppress non-radiative pathways and inner-filter effects, and facilitate surface-trap passivation, resulting in substantially enhanced Förster resonance energy transfer (FRET). The engineered FRET composites exhibit efficient and stable white-light emission with chromaticity characteristics approaching midday sunlight and photostability exceeding one month. Furthermore, ratiometric fluorescence-based sensing enables ultrasensitive detection of synthetic food colorants at nanomolar concentrations. A $Zn^{2+}$-directed PFN comprising HQS-stabilized Ag nanoparticles and ZQC exhibits plasmon-enhanced fluorescence, ppb-level detection of nitroaromatic pollutants, synergistic antibacterial activity, and efficient cellular imaging. The PFN further integrates environmental sensing, antimicrobial performance, and bioimaging within a single stable multifunctional platform with enhanced optical stability and biological compatibility. Collectively, these findings establish interfacially engineered QDC and PFN architectures as multifunctional nanomaterials for advanced solid-state lighting, food and environmental monitoring, antimicrobial applications, and biomedical imaging.

**Keywords:** Quantum dots; Förster resonance energy transfer; plasmonic-fluorescent nanocomposites; white light emission; sensing; antimicrobial activity; bioimaging.

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# Understanding Chemical Mechanisms Through Molecular Spectroscopy

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PM Research group works in the field of gas-phase chemical physics, specifically in molecular spectroscopy and its allied areas. Molecular spectroscopy gives insight into the nature of the potential energy surface and the myriad ways in which quantized states (electronic, vibrational, rotational, hyperfine) interact with each other. The two components of a spectrum, frequency and intensity, encode mechanistic details of dynamical processes including collisional energy transfer, isomerization reaction, and photodissociation. A few interesting examples of extracting dynamical information from high-resolution spectroscopy will be discussed, including the mechanism of photodissociation of *symmetric*-Triazine and energy transfer during an atom-molecule collision. Related ongoing projects including introducing new techniques in gas-phase spectroscopy, Fischer-Tropsch synthesis, aerospace combustion, ablation of meteorite analogs, modelling of collisional energy transfer, and computational astrochemistry will be shown.

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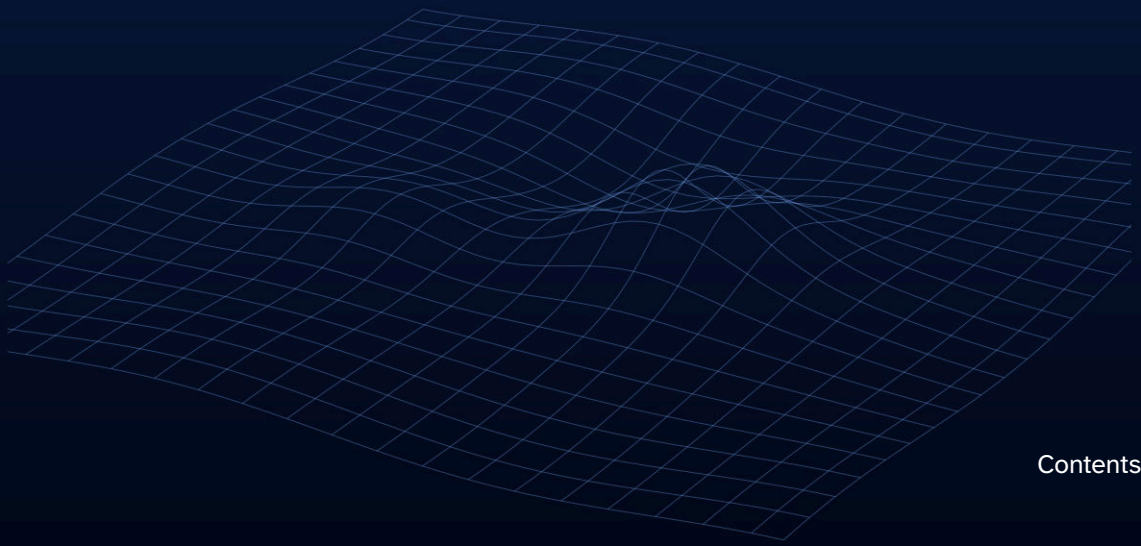
**Keywords:** High-resolution spectroscopy; Chemical dynamics; Technique development

ABSTRACTS

# Special Evening Lectures

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# From Molecular Chirality to Living Helices: Symmetry Breaking, Cooperativity, and Handedness Selection

Biman Bagchi
Solid State and Structural Chemistry Unit
Indian Institute of Science, Bengaluru, India

**Abstract**

The 2026 Nobel Prize in Chemistry to Henri Kagan and Kenso Soai has brought renewed attention to one of nature's most fascinating phenomena: molecular chirality and the amplification of handedness. Chirality is intimately connected with optical activity, asymmetric chemical synthesis, and the molecular organization of living systems. Biology exhibits a remarkable preference for L-amino acids and D-sugars, while proteins and DNA organize into predominantly right-handed helices. How does molecular asymmetry lead to such large-scale structural order? And can a helical structure emerge even when its molecular constituents are achiral? In this lecture, I shall explore these questions using simple ideas from statistical mechanics, polymer physics, and physical chemistry. We begin with the diverse morphologies of semiflexible polymers, where competition among entropy, attraction, and bending stiffness produces coils, globules, rods, and toroids. Helices, however, are special: their formation requires additional geometric constraints or cooperative molecular interactions. We discuss how helical segments nucleate, grow, fluctuate, and disappear, giving rise to transient structures that we call *living helices*. A further question concerns the selection and persistence of handedness in these fluctuating structures. A simple three-state statistical-mechanical model reveals that the persistence of helical order and the persistence of chirality are governed by distinct correlation lengths. Finally, we examine how weak molecular chiral preferences can be amplified through cooperative interactions, and how collective chirality can emerge spontaneously in molecular assemblies. The lecture connects the Nobel-winning discoveries in asymmetric chemistry with the statistical mechanics of helices in polymers and biopolymers.

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**Deep tech in photonics needs talent, ideas, resources, AND deep experience: let's put them together**

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With the geo-political turmoil upon us, the time has come for capable scientists to deliver advanced technology. For India to succeed in photonics deep-tech, we need to put together expertise from different areas: lasers, detectors, fibers, optics, mechanics, fast electronics and AI/ML-based data analysis. Such expertise will have to come from our best academic labs, which have the responsibility to dream up and construct devices that are not cheaper, not 'import substitutes', but are simply better than anything that exists anywhere. As an example, I will talk about our recent success in making a medical imaging device for digital pathology.

Mark Maroncelli
Penn State University, USA


# Adventures of a Lonely Water Molecule as Told by IR, FIR, NMR Spectroscopy and MD Simulation

Mark Maroncelli, Kallol Mukherjee, and Sourav Palchowdhury

Absent sufficient care, most solvents, especially ionic liquids, contain some amount of water. Partly for its intrinsic interest, and partly to serve as an extreme limit of currently popular water-in-salt electrolytes, we have been studying “solitary” water, water at sufficient dilution that water-water interactions are absent. In this limit, the solvation structure, energetics, and dynamics of water are determined only by water-solvent interactions. The frequencies of OH-stretching bands of solitary water are strongly correlated to the hydrogen-bond accepting ability of solvents, with the same correlation applying to both ionic and dipolar liquids. The OH bands of $H_2O$ exhibit complex structure, typically requiring 4-5 components to accurately describe their shapes. Molecular dynamics simulations show this substructure stems from an underlying distribution of hydrogen bonding motifs present in polar solvents. Water’s dynamics play an important role in transforming the inhomogeneous distribution of frequencies created by these motifs into the observed band shapes. In contrast, far-infrared (FIR) bands of solitary water are mostly unstructured. Simulations show the FIR spectrum simply reflects water’s rotational motions, which range from quasi-free rotation in nonpolar solvents like $CCl_4$ to highly constrained libration in ionic liquids with charge-dense anions. FIR band frequencies, which correlate with OH frequencies, are found to provide a direct measure of the torques the solvent imposes on water rotations. The link between such torques and related forces and the transport of water in different solvents were finally established using NMR measurements of water rotation times and translational diffusion coefficients.

ABSTRACTS

# Invited Faculty Posters

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22 abstracts

# Investigation of conformational dynamics and ligand binding mechanism of gene regulatory SAM-II / SAM-V tandem riboswitch

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Riboswitches are short, 5'-non-coding sequences in bacterial mRNA which regulate transcription/translation of the downstream genes upon binding of specific cellular metabolites [1]. S-adenosyl methionine (SAM) is an important metabolite that binds to six different classes of SAM-riboswitches. Breaker and coworkers identified a tandem SAM-II/SAM-V riboswitch arrangement in which an upstream transcriptional SAM-II riboswitch and a downstream translational SAM-V riboswitch regulate the same *bhmt* gene [2]. To understand the molecular mechanisms of gene regulation by this tandem riboswitch, here we study the folding-unfolding dynamics of the ligand binding 'aptamer' domains of individual SAM-II and SAM-V riboswitches, as well as their ligand (SAM) and co-factor ($Mg^{2+}$) binding properties using Förster resonance energy transfer (FRET).

By performing two-dimensional fluorescence lifetime correlation spectroscopy (2D FLCS) [3, 4], we observe that both SAM-II and SAM-V aptamers undergo conformational switching between a low-FRET 'hairpin' structure and high-FRET 'pseudoknot' structure on the microsecond-millisecond time scale (Figure 1). In the apo form, i.e., in the absence of ligand and cofactor, both aptamers predominantly exist in the hairpin structure. Upon binding of $Mg^{2+}$ with similar affinities – dissociation constants, $K_d$ ~ 3-4 mM – both aptamers transition to the pseudoknot structure. Binding of SAM in the absence of $Mg^{2+}$ also transitions both aptamers from hairpin to pseudoknot structures, however at vastly different concentration ranges of SAM – with $K_d$ ~ 20 µM for SAM-II aptamer and $K_d$ ~ 1.5 mM for SAM-V aptamer. Interestingly, the presence of physiologically relevant 2 mM $Mg^{2+}$ facilitates the binding of SAM to both aptamers by ~30 times – with $K_d$ ~ 700 nM and ~ 50 µM for SAM-II and SAM-V aptamers, respectively. Our results suggest that the two riboswitches likely perform gene regulation at different cellular levels of SAM: SAM-II riboswitch regulates transcription at nano-micromolar concentrations of SAM, whereas SAM-V riboswitch regulates translation at micro-millimolar concentrations of SAM.

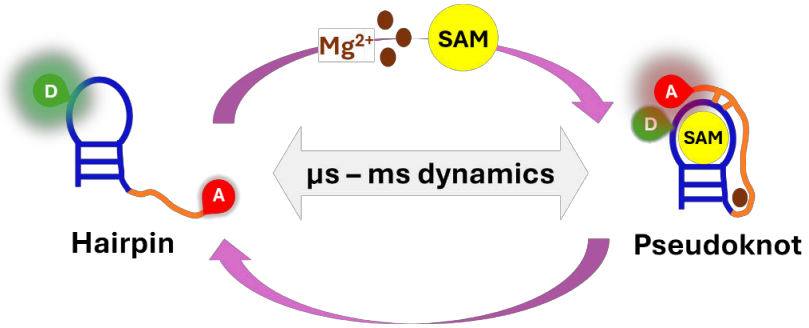



**Figure 1.** Schematic illustration of hairpin - pseudoknot conformational dynamics of SAM-II and SAM-V aptamers.

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**Keywords:** SAM riboswitch; Gene regulation; 2D FLCS

# Mapping Conformational and Kinetic Landscapes of 14-3-3σ/α-Synuclein Assembly via Variational Autoencoders and Markov State Models

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The interaction between the molecular chaperone 14-3-3σ and the intrinsically disordered protein α-synuclein is implicated in the pathogenesis of Parkinson's disease, yet its dynamic mechanism remains poorly understood at an atomistic level. The inherent flexibility and rugged energy landscape of this complex pose significant challenges to conventional molecular dynamics simulations. Here, we employ an advanced adaptive sampling framework that integrates variational autoencoders (VAEs) and Markov state models (MSMs) to overcome these limitations and obtain comprehensive atomistic insight into the 14-3-3σ/α-synuclein assembly. Our VAE-driven approach iteratively learns a low-dimensional latent space of the system's dynamics, guiding simulations to efficiently explore and sample novel conformations. This strategy successfully captured over 90% of the conformational variance observed in a 17 μs reference trajectory using around 3 μs of simulation time. An MSM constructed from approximately 20 μs of combined simulation data revealed three key metastable states: a highly stable bound complex, a structurally distinct intermediate, and a disordered, largely unbound ensemble. The resulting kinetic model quantitatively characterized the transition pathways, identifying the final bound state as a deep kinetic trap with a dissociation time scale of over 100 μs, confirming its high stability. Furthermore, we elucidated the crucial role of the intermediate state as a primary steppingstone in the dissociation pathway. This work not only provides valuable atomistic insight into a key interaction relevant to neurodegeneration but also establishes the VAE-MSM pipeline as a powerful tool for dissecting the complex mechanisms of disordered protein-protein interactions.

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**Keywords:** Parkinson's Disease, Protein-Protein Interactions, Variational Autoencoders, Markov State Models.

# CMA−ES-based Force Field Parameter Optimization of Diiodomethane for Surface Free Energy Calculations

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Surface free energy (SFE) is a fundamental property governing the wettability of solid surfaces and is commonly determined indirectly using probe liquids with known surface tension components. Diiodomethane is widely used as a dispersive probe liquid for SFE determination because of its high surface tension and predominant dispersive character. However, experimental determination of SFE can be challenging due to surface impurities, roughness, and contact angle hysteresis, which can introduce uncertainties in the measured contact angle. Molecular dynamics (MD) simulations provide an alternative approach that can avoid these experimental complications by allowing the solid–liquid interface to be studied under controlled conditions. However, commonly used force fields such as AMBER, CHARMM, and OPLS substantially underestimate the surface tension of diiodomethane at room temperature. In this study, we optimized OPLS-based force field parameters[1] for liquid diiodomethane using the covariance matrix adaptation evolution strategy (CMA-ES)[2] through three different parameter optimization workflows, involving either initial manual tuning followed by CMA-ES optimization or direct optimization of selected or all parameters using CMA-ES. All three parameter sets closely reproduce the experimental surface tension of 49.69 $\mathrm{mN,m^{-1}}$ at 298 K. The optimized models were further assessed using diiodomethane–water interfacial tension, dielectric constant, temperature-dependent surface tension and density, and vapor–liquid coexistence properties. Overall, the three parameter sets exhibit comparable performance across the investigated properties and closely match the experimental results. We further estimate the surface free energy of graphene and graphite and compare the results with experimental values[3−4]. The diiodomethane models presented in this study can be used as test liquids to estimate the SFE of polymer-coated surfaces, self-assembled monolayers (SAMs), and high-energy surfaces such as metals and ceramics.

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**Keywords:** Diiodomethane force field; CMA-ES optimization; Contact angle, Surface free energy

# Breaking Azeotropes: The Role of Entrainers in Efficient Separation

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Azeotropic mixtures are challenging to separate by conventional fractional distillation because their liquid and vapor phases have identical compositions at the azeotropic point. This limitation is particularly important in chemical and pharmaceutical industries where high purity component recovery is required. Entrainers are therefore introduced to modify intermolecular interactions and vapor–liquid equilibrium, enabling more effective separation of the original components. However, selecting a suitable entrainer through experimental methods alone is time-consuming and expensive. Molecular dynamics (MD) simulation offers an efficient approach for understanding entrainer–component interactions at the molecular level.

In this study, the effects of the ionic liquid 1-ethyl-3-methylimidazolium chloride ([EMIM]Cl) and benzene on the hydrogen-bonding structure and diffusion behaviour of the ethanol–water azeotrope were investigated. The results show that [EMIM]Cl interacts more strongly with both ethanol and water than benzene, leading to a faster reduction in same-species and cross-species hydrogen bonding. In addition, [EMIM]Cl decreases the diffusion coefficient of water more significantly than that of ethanol, indicating stronger selective interactions with water. These findings suggest that [EMIM]Cl is a more effective entrainer than benzene for disrupting the ethanol–water azeotrope and may support the design of improved azeotropic separation processes.

**Keywords:** Azeotrope, Entrainer, Ionic liquid, Molecular dynamics simulation, Hydrogen bonding

# Activation of atomically precise monolayer-protected Pt nanoclusters: Formation of active CO oxidation catalysts

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In the past few decades, there has been substantial interest in developing noble metal nanoparticle (supported on metal oxides) based industrial catalysts for pollutant control. However, recent global developments require further reduction in the total amount of noble metals used in these catalysts. Atomically precise Pt nanoclusters, co-protected by CO and triphenyl phosphine (TPP) ligands, e.g. $[Pt_{17}(CO)_{12}(TPP)_8]^{2+}$, forms active catalyst for CO oxidation upon removal of the protecting ligands.[1,2] However, the changes occurring to the cluster upon thermal activation during the formation of the active catalyst are poorly understood. We used a combination of hybrid mass spectrometry and surface science to map the mechanism and energetics of thermal activation of $[Pt_{17}(CO)_{12}(TPP)_8]^{2+}$ cluster in the gas-phase and on inert supports in the condensed-phase.[3] In both cases, a characteristic sequence of CO and benzene desorption steps was observed, followed by $H_2$ loss at higher excitation energy. High-resolution mass and ion mobility spectrometry together with DFT-based modelling were used to probe the sequence of fragmentation reactions and fragment structures generated upon collisional excitation of $[Pt_{17}(CO)_{12}(PPh_3)_8]^{2+}$.[3] In addition, we study the effect of metal oxide supports and varying activation conditions on the activity of the catalyst formed by ligand removal from the precursor nanocluster.

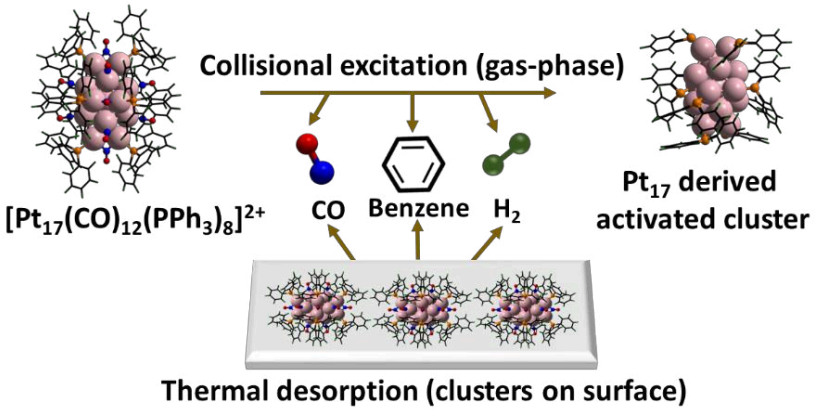



**Figure 1.** Schematic showing the activation of the cluster in the gas-phase and in the condensed phase [3]

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**Keywords:** clusters; nanocatalysis; mass spectrometry; surface science

# Machine Learning Approach to Screen Potential Donor and Acceptor Fragments: Insights from Chemical Reactivity

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Density functional theory has given us a rigorous methodology to understand the chemical reactivity via global and local reactivity parameters. However, high computational cost make it difficult to design efficient solar cells at less time in this rapid growing world. Machine learning approach enables screening of efficient donor and acceptor molecules from huge space without expensive computation and just by learning the pattern. Here we have implemented the intuition of global reactivity parameters to screen optimal donor and acceptor molecule using machine learning algorithms. Throughout this study it has been uncovered that the chemical reactivity of the individual donor and acceptor fragment are highly impactful for device level efficiency that guides to design novel candidates for future. Almost forty-two ML models are tested, among which random forest regression, light gradient boosting machine regression, and Nu support vector regression models appear to be the best models. The solar cell device performance defined by the device properties, *i.e.,* photoconversion efficiency, short circuit current, open circuit voltage and donor and acceptor molecule's charge transfer are predicted using best machine learning model. Potential donor and acceptor fragments have been screened by multiobjecitve optimization of chemical reactivity and synthetic accessibility score by taking into consideration of high solar cell efficiency. This strategic ML framework is able to find the efficient donor and acceptor counterparts based on its chemical stability that directly influence solar cell performance, in short time and in an efficient way.

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**Keywords: Chemical reactivity parameter; Machine learning regression model; Solar cell**

# Exploring Toehold-Independent DNA Strand Displacement through Parallel Triplex Formation

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DNA triplex formation offers an alternative strategy for nucleic acid strand displacement reactions (SDRs), potentially enabling molecular systems with reduced dependence on conventional toehold domains. However, the stability, sequence specificity, and kinetic behavior of triplex-mediated SDR remain important challenges. In this study, circular dichroism (CD) spectroscopy, ensemble fluorescence measurements, and gel electrophoresis were employed to investigate the effects of divalent and monovalent cations, duplex precursor length, sequence mutations, and output-strand overhangs on parallel DNA triplex formation and triplex-mediated SDR. CD measurements revealed that $Mg^{2+}$ plays a critical role in stabilizing the parallel triplex, whereas $Na^{+}$ provides insufficient stabilization under the investigated conditions. A 20-nucleotide duplex precursor supported the formation of a 12-nucleotide parallel triplex more effectively than a 12-nucleotide precursor, suggesting that the additional duplex region contributes to triplex stabilization. Ensemble fluorescence measurements further demonstrated the essential role of $Mg^{2+}$ in promoting triplex-mediated strand displacement. Notably, increasing $Mg^{2+}$ concentration enhanced reaction kinetics even when the corresponding CD signatures were similar, highlighting the greater utility of product-linked fluorescence measurements for assessing functional triplex-mediated displacement. Mutational analyses revealed position- and potentially length-dependent sequence specificity: mutations at internal positions of a 12-nucleotide triplex-forming domain (TFD) substantially reduced reaction rates, whereas mutations near its terminus had comparatively limited effects. However, mutations at the terminal region of a shorter, 10-nucleotide TFD significantly affected reaction kinetics, suggesting that sequence recognition depends on TFD length. Furthermore, triplex-mediated SDR proceeded in the absence of an output-strand overhang, although with reduced reaction rates and altered kinetic behavior, unlike conventional toehold-mediated SDR, which requires an accessible toehold for initiation. Despite its slower kinetics and requirement for acidic conditions (pH 5), triplex-mediated SDR offers a potentially less leaky and less enzyme-accessible alternative to conventional toehold-mediated systems. These findings establish key physicochemical and sequence-dependent determinants of triplex-mediated strand displacement and provide insights for the design of alternative DNA-based molecular reaction systems.

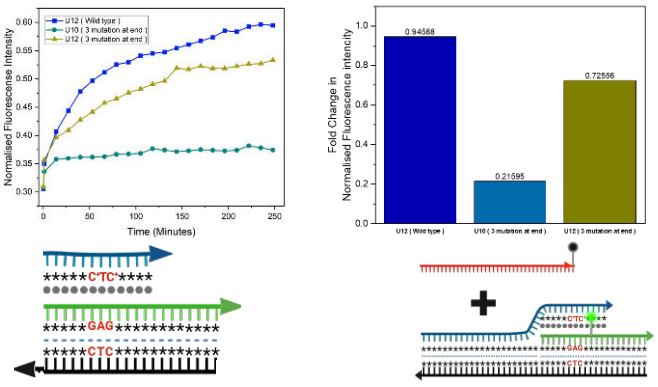



Fig: Mechanism of triples formation through Toe-less mechanism

# Physics-Informed Machine Learning for Enzyme Catalysis

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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, 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] (Figure 1). The resulting framework has proven to be fast, accurate, and transferable, making it a promising platform for rational enzyme engineering and drug design.

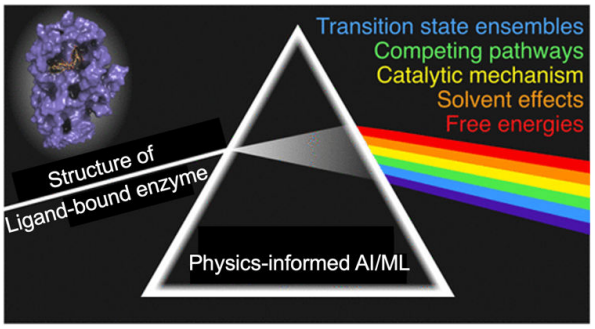



**Figure 1.** Input and outputs in the physics-based ML protocol for enzyme catalysis.

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**Keywords:** transition state; drug discovery; free energy; kinetics; transferable machine learning

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# Mode-Dependent Vibrational Energy Flow in Hydrogen-Bonded Dimers: A Unified Mechanism for Intramolecular Vibrational Energy Redistribution and Vibrational Predissociation

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Hydrogen-bonded complexes exhibit distinct relaxation pathways depending on the initially excited local vibrational mode. Using phenol and water dimers as prototypical systems, we show that donor O-H stretching excitation leads to faster intramolecular vibrational redistribution (IVR) but slower predissociation, whereas acceptor O-H excitation preferentially transfers energy into intermolecular hydrogen-bond modes, accelerating dissociation, which aligns well with the experimental findings of the phenol dimer. We attribute this asymmetry to geometric constraints on the donor over acceptor O-H groups. Consistent with this interpretation, the structurally constrained acceptor in the sulforaphane-cysteine complex exhibits the opposite coupling pattern. A reduced Hamiltonian including donor O-H, acceptor O-H, and hydrogen-bond coordinates with harmonic and anharmonic couplings, generated from the molecular geometries, successfully reproduces the IVR and predissociation dynamics observed in the simulations. This identifies the key coupling terms governing the competing relaxation pathways and suggests that donor-acceptor coupling asymmetry is a general feature of hydrogen-bonded systems.

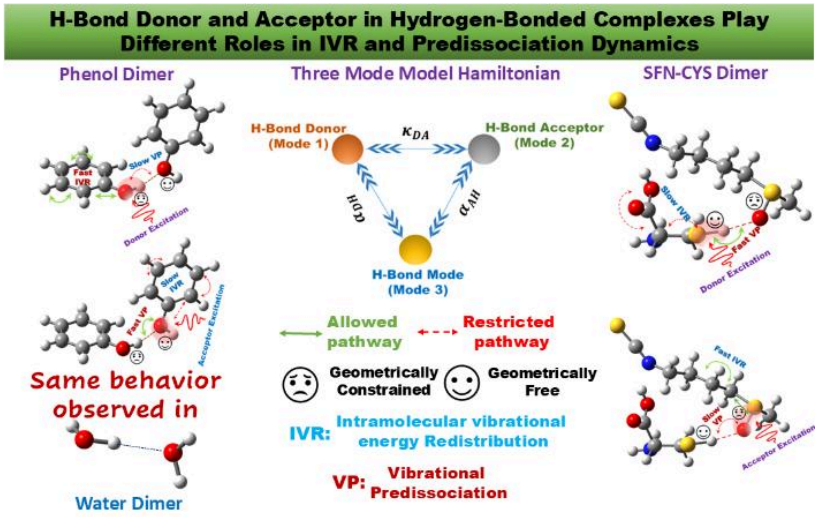



**Figure 1.** Schematic diagram showing different dynamics of OH-acceptor and OH-donor sites

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**Keywords:** IVR; OH-acceptor; OH-donor; Reduced Hamiltonian.

# Decoding the Molecular Interactions of Thymol, Thymoquinone, and Lawsone with DNA and Protein: Experimental & Computational Approach

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Three bioactive phytochemicals, namely thymol (Tl), thymoquinone (TQ), and lawsone, derived from *Thymus vulgaris*, *Nigella sativa* seeds, and *Lawsonia inermis* leaves, respectively, were investigated for their binding affinities toward calf thymus DNA (CT-DNA) and bovine serum albumin (BSA) using experimental and computational approaches. The binding phenomenon was carried out using several spectroscopic techniques like absorbance, fluorescence, and circular dichroic spectroscopy. Spectroscopic studies revealed that all three compounds have a high affinity towards both the receptors, DNA and BSA. These phytochemicals bind to the minor groove of DNA and suitable hydrophobic pockets of BSA. The binding affinities are in the range of $10^5 M^{-1}$ for both DNA and BSA with all three phytochemicals. To understand the excited state behaviour of these molecules, time-resolved fluorescence experiment was done. TQ and Lawsone show three exponential decays in solvents with varying polarity with a fast dynamic of time constant ~18 ps with amplitude ~90–98%. The emission intensity of BSA was quenched due to the binding with studied molecules. The quenching mechanism for TQ and Tl is mainly due to static mode, while the quenching for lawsone was due to both static and dynamic contributions. Isothermal titration calorimetric (ITC) study was carried out to understand the thermodynamic behaviour during the interaction. The binding was mainly favoured by negative enthalpy changes. Experimental results were validated using molecular docking study and were observed that all three molecules bind to the minor groove of DNA and to Sudlow's site I in Domain II and sub-domain IIA of BSA. Both experimental and computational findings highlight the significance of structural variation on binding affinities.

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**Keywords:** Phytochemicals; DNA/BSA binding; spectroscopy; time-resolved fluorescence; molecular docking

# Active Polymers in Porous Media: Activity-Driven Conformational and Transport Dynamics

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Active Polymers represent a distinct class of non-equilibrium systems whose structure and movement are profoundly influenced by the nature of activity and environmental complexity [1,2,3,4]. This study uses Brownian Dynamics simulations to compare the behavior of Active Brownian (ABPC) and Tangentially Active (TAPC) polymer chains within a 2D porous medium. Our results reveal distinct conformational and dynamical differences between the two models. While ABPC undergoes unrestrained motion at high activity, TAPC exhibits reptation-like motion at lower activity, enabling efficient escape from structural traps but undergoes spiraling at high activity. We hope our study will motivate experimentalists to design active smart materials with a task of navigating through complex environments.

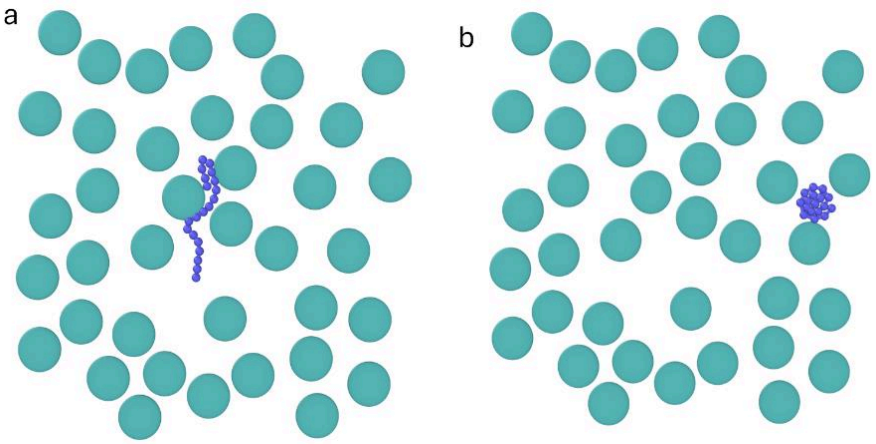



Figure 1: Representative simulation snapshots of ABPC (a) and TAPC (b) in porous media.

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**Keywords:** Active Polymers; Porous Media; Brownian Dynamics; Non-equilibrium systems

# Quantifying the Intrinsic Energetic Thresholds of Solvent-Driven Excited-State Proton Transfer

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Directly measuring the exact reaction energy barrier of excited-state proton transfer (ESPT) pathways remains a persistent challenge due to transient photoproducts and rapid quantum tunneling effects. To overcome these limitations, we report a multi-resonance laser spectroscopic approach to map the exact $S_1$ excited-state potential energy landscape in isolated 1:1 water complexes of 2-(2′-pyridyl)-benzimidazole (PBI). By combining mass-selective two-color resonant two-photon ionization (2C-R2PI), ion-dip infrared (IDIR), and UV-UV hole-burning spectroscopies in a supersonic jet-cooled molecular beam, we successfully bypassed ultrafast ionization signal dropout to capture the hidden vibronic transitions at the reaction threshold.

By evaluating site-specifically deuterated isotopomers, we bracketed the experimental activation barriers at 666 ± 16 $cm^{-1}$ for the chromophore-deuterated PBI(D)-$H_2O$ and 935 ± 40 $cm^{-1}$ for the solvent-deuterated PBI-$D_2O$. This highly asymmetric barrier escalation upon solvent deuteration definitively demonstrates that the proton-transfer reaction coordinate is predominantly solvent-driven, ruling out a concerted hydrogen atom transfer pathway. Furthermore, our experimentally bracketed thresholds exhibit remarkable quantitative agreement (within a 0–6% error margin) with zero-point energy-corrected, dispersion-corrected density functional theory (B3LYP-D4) and CASPT2 calculations. Ultimately, this integrated experimental and computational template demonstrates that heavy-isotope substitution effectively suppresses light-atom quantum tunneling, isolating the purely classical potential energy landscape and providing a robust framework for capturing transient bond rearrangements at the single-molecule level.

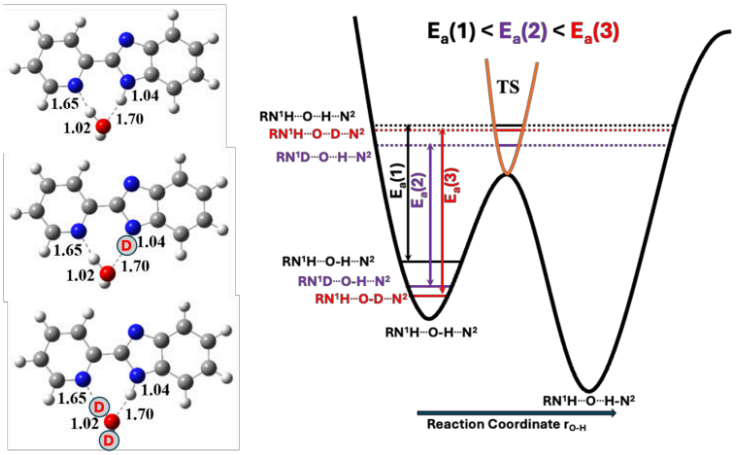



**Figure 1. Selective** isotopic substitution an d its effect on reaction energy barrier

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**Keywords:** Reaction energy barrier; isotopic substitution; quantum tunnelling

# Regulation of Protease Activity of Papain via Biomolecular Condensation and Its Reactivation by L-Cysteine

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Proteases are enzymes that break down proteins and play essential roles in biological processes and industrial applications. Understanding how protease activity can be switched between active and inactive states is important for controlling their function. Here, we demonstrate that the protease activity of papain can be regulated through spontaneous liquid–liquid phase separation (LLPS) [1], in which dissolved papain molecules spontaneously condense into protein-rich droplets under macromolecular crowding conditions. We show that macromolecular crowding promotes papain condensation through intermolecular hydrophobic interactions, accompanied by a more compact protein conformation and an increased α-helical content. While free papain efficiently hydrolyzes synthetic and protein substrates, papain condensates exhibit markedly reduced proteolytic activity toward protein substrates. We further demonstrate that this dormant state is associated with intermolecular disulfide-bond formation involving the catalytic cysteine residue Cys25 between neighboring papain molecules within the condensed phase. Importantly, treatment with the naturally occurring amino acid L-cysteine restores papain activity, consistent with thiol–disulfide exchange and regeneration of the catalytically active thiol state, resulting in more uniform soluble peptide fragments. Our findings reveal a previously unrecognized connection between protein condensation, conformational compaction, and reversible regulation of protease activity. This work provides a molecular framework for understanding how phase separation can modulate enzyme function and suggests a potential strategy for controlling papain activity in biotechnological and food-processing applications, including meat tenderization.

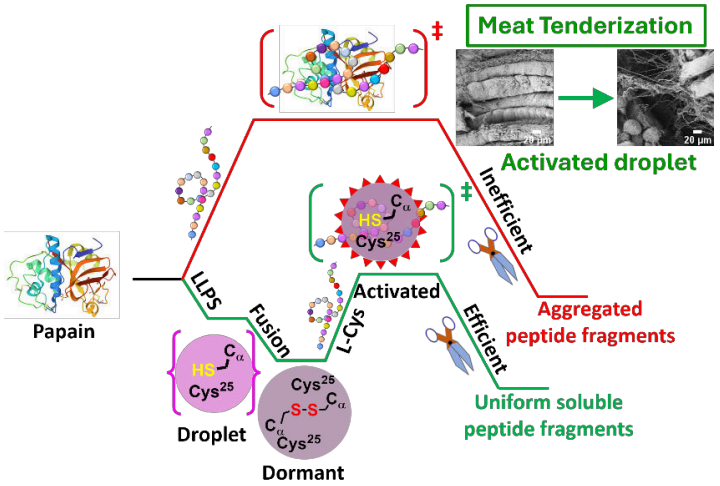



**Figure 1. Spatio-temporal regulation of protease activity of papain via LLPS and L-Cysteine activation.**

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**Keywords:** proteases; papain; macromolecular crowding; phase-separation

# Multiscale Modeling of Electrochemical Catalysis and Energy Storage Systems via Molecular Dynamics Simulations

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Molecular-level insights into energy storage materials and electrocatalytic interfaces are required to accelerate the transition toward energy demand. The experimental approach may not be suitable for exploring the expansive chemical space of complex catalytic environments and rechargeable battery components. Here, we present a unified computational framework that combines first-principles molecular dynamics (FPMD), classical simulations, and machine-learning (ML) potentials to model and design advanced materials for energy storage and conversion. Our research area focuses on two major verticals: solid-state battery electrolytes/electrodes and electrochemical catalysis for small-molecule activation. [1] Using atomistic simulations, we evaluate ionic transport mechanisms in the solid and liquid states, interfacial stability, and intercalation kinetics in electrolyte and electrode systems. By incorporating machine-learning potentials trained on Density Functional Theory (DFT) data, we achieve near-quantum-accuracy over extended spatial and temporal scales, enabling precise tracking of dynamic ion diffusion pathways and structural phase transformations.[2] In parallel, we employ constant-potential molecular dynamics to capture the real-time dynamics of catalytic interfaces under explicit reaction conditions. [3] This approach provides mechanistic insights into solvent-electrolyte structuring, local electric field fluctuations, and microkinetic reaction pathways at the electrode boundary. Furthermore, we apply inverse design protocols to rapidly screen tailored ionic liquid formulations and optimized electrode architectures with targeted transport and catalytic performance metrics. By bridging quantum mechanics, neural network force fields, and statistical thermodynamics, our work provides design principles for next-generation energy storage media and electrocatalysts. The integration of various advanced methods offers a scalable strategy to bypass conventional trial-and-error discovery, paving the way for targeted material synthesis for clean energy applications.

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**Keywords:** Constant Potential Molecular Dynamics, Heterogeneous Electrocatalysis, Ionic transport, Metal-ion Battery, Electrode, and Electrolyte

# Conductivity in Battery Electrolyte Systems: Impact of Ultrafast Solution Dynamics, Ion-Ion Motional Correlations, and Solution Heterogeneity

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## Abstract

A comprehensive understanding of ion transport in battery electrolyte systems requires elucidating the roles executed by ultrafast solution dynamics, motional correlations of among the transporter ions, and spatiotemporal heterogeneity of the solution [1,2]. We have studied several such systems, both via theoretical + computational and experimental techniques, and gained several important understanding regarding the roles of these solution aspects [3]. The role of water structure and residence times in the proximity of ions have also been found to play critical roles in controlling conductivity in aqueous systems [2], while cosolvent's influence has been investigated in determining the optimal composition of a given binary host system [4]. Formation of ion-pairs and ion-aggregates, and their effects along with the impact of spatiotemporal heterogeneity of ionic solutions on conductivity in these systems have also been ascertained [1,5,6]. Some of these results will be presented and the physical chemistry aspects discussed in this presentation.

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**Keywords:** Battery electrolyte systems, ultrafast solution dynamics, motional correlations, heterogeneity

# Navigating Pathways in Free Energy Landscape: Adaptive (Machine) Learning Strategies Towards Rare Event Kinetics

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## ABSTRACT

Computation of the underlying free energy landscapes for any complex chemical or biophysical processes provides quantitative insights into the thermodynamics and kinetics of the process, including the mechanistic pathways. However, several important (bio)chemical processes occur on timescales not accessible to standard computational methods like atomistic molecular dynamics (MD) simulations. This motivates the development of enhanced sampling methods to accelerate rare events. However, identification of suitable reaction coordinate(s) or a mechanistic hypothesis is crucial to the success of such methods.

In this talk, we shall discuss a few computational methods developed in our group for adaptive navigation of rugged energy landscapes to generate reactive pathways. We shall demonstrate how we can efficiently compute rare event kinetics, e.g. drug unbinding kinetics (residence time; $k_{off}$), which is an effective parameter in drug discovery research, at a reasonable computational cost.

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# Resonantly Stabilized Free Radical Mediated Mass Growth: Indenyl Chemistry as the Common Thread of Planar and Curved PAHs

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Polycyclic aromatic hydrocarbons (PAHs) - fused-ring carbon compounds analogous to naphthalene and larger relatives are widely regarded as molecular precursors to carbonaceous nanoparticles, soot, and ultimately carbon-rich dust throughout the galaxy. Such species have now been identified directly in cold molecular clouds (TMC-1), in the Murchison meteorite, and in returned samples from the carbonaceous asteroids Ryugu and Bennu, yet how their carbon skeletons assemble and grow under the extreme, low-density conditions of circumstellar envelopes and combustion flames has remained poorly understood, particularly since the emergence of resonantly-stabilized free radical (RSFR)-mediated pathways as an alternative to stepwise acetylene addition.[1]

Our recent microreactor pyrolysis experiments probed by synchrotron vacuum ultraviolet (VUV) single photon ionization mass spectrometry in combination with electronic structure calculations show that the aromatic, resonantly-stabilized 1-indenyl radical ($C_9H_7^{\bullet}$), bearing a cyclopentadienyl-fused six-membered ring undergoes barrierless or near-barrierless self- and cross-recombination to isomer-selectively build significantly larger PAHs. Indenyl self-recombination, proceeding through pivotal spiroaromatic intermediates and ring expansion of the five-membered moiety, yields the planar, 18π-Hückel-aromatic PAH chrysene ($C_{18}H_{12}$) in an overall endoergic step, rationalizing its detection in pristine Ryugu and Murchison samples.[2] Cross-recombination of indenyl with the benzyl radical ($C_7H_7^{\bullet}$) instead proceeds via C–C bond formation, cyclization, and dehydrogenation to fluoranthene ($C_{16}H_{10}$), a non-alternant, five-membered-ring-bearing PAH also identified in Ryugu and Bennu material, and a structural link toward curved carbon nanostructures such as fullerenes and nanotubes.[3] Together, these findings establish indenyl-radical recombination as a single, versatile mass-growth channel spanning planar graphene-type and curved non-alternant PAHs, offering a unified mechanistic framework for carbon-network assembly in circumstellar envelopes, planetary nebulae, and terrestrial flames.

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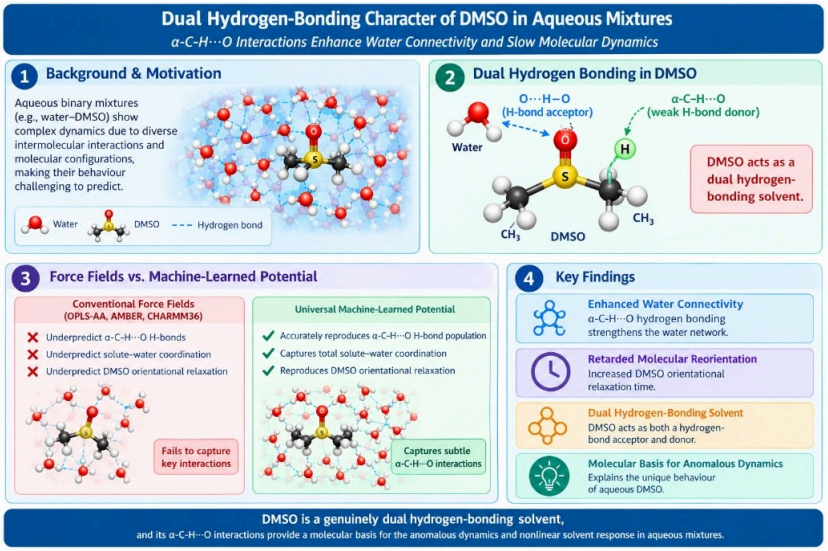
**Keywords:** Radical recombination; PAH growth; Indenyl radical; Astrochemistry; Curved carbonaceous architecture.

# Beyond the Sulfoxide Oxygen: NMR Spectroscopy and Machine-Learned Dynamics Reveal α-C–H···Ow Hydrogen Bonding in Dimethyl Sulfoxide-Water

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Owing to the greater diversity of intermolecular interactions and molecular configurations, aqueous binary mixtures exhibit complex dynamical behaviour that is often absent in pure liquids, making their behaviour challenging to understand and predict and attracting considerable interest in recent years. Among these systems, water–dimethyl sulfoxide (DMSO) mixtures are particularly intriguing because of their distinctive physicochemical properties and broad relevance to chemistry and biology. Dimethyl sulfoxide (DMSO) is conventionally regarded as a strong hydrogen-bond acceptor, whereas the role of its acidic α-C-H groups as weak hydrogen-bond donors remains unresolved and, interestingly, exhibits a series of intriguing yet unexplained anomalies. We combine NMR spectroscopy, fluorescence anisotropy, and molecular dynamics simulations using a universal machine-learning potential to probe the α-C-H···O hydrogen-bonding channel, a key determinant of aqueous DMSO dynamics. The latter required many simulations to obtain a reliable average. We carried out systematic molecular dynamics simulations of the water–DMSO mixture using several widely employed force fields and found that conventional approaches, including OPLS-AA, AMBER, and CHARMM36, substantially underpredict the α-C–H···O hydrogen-bond population, total solute–water coordination, and DMSO orientational relaxation, thereby failing to capture this interaction. In contrast, a universal machine-learned potential accurately reproduces these features, highlighting its ability to describe the subtle α-C–H···O hydrogen-bonding interactions in aqueous DMSO. Together, these results reveal that weak α-C–H···O hydrogen bonding enhances water connectivity and retards molecular reorientation, providing a molecular basis for the anomalous dynamics of aqueous DMSO and establishing DMSO as a genuinely dual hydrogen-bonding solvent. This dual hydrogen-bonding character also manifests as a pronounced nonlinear solvent response, reflected in substantially different responses of the solute probe indole in its ground and excited states as well as in nonequilibrium solvation, with the effects being most pronounced in the 20–35% DMSO concentration regime.




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**Keywords:** Water–DMSO mixtures, α-C–H···O hydrogen bonding, Molecular dynamics simulations Machine-learning potential

# A multiscale study in search of photoswitchable drug for serotonin receptors

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Serotonin receptors regulate diverse neurological processes, including mood, sleep, appetite, cognition, learning, and memory [1–3]. Azobenzene-based photoswitchable ligands offer a promising strategy for controlling receptor activity with light. Here, we investigated trans azobenzene-fused serotonin (TAS) and cis azobenzene-fused serotonin (CAS) bound to the 5-$HT_{1B}$ receptor using quantum chemical calculations, molecular dynamics simulations, enhanced sampling simulations and free-energy calculations. Our results show that TAS has a more favorable thermodynamic binding affinity than CAS, with the lipid membrane significantly influencing the relative stability of the two receptor–ligand complexes.[4] In contrast, umbrella-sampling simulations indicate that CAS exhibits slower unbinding kinetics, suggesting that photoisomerization from TAS to CAS can prolong receptor-bound states. Quantum chemical calculations further demonstrate that fusion of azobenzene with serotonin modifies the potential-energy surface and may influence photoswitching kinetics. Ground-state energy barriers for cis-to-trans thermal back-isomerization were also evaluated in the receptor, solvent, and gas phases to assess the stability of the photoswitched state. Together, these results provide molecular-level insights into the thermodynamic, kinetic, and photochemical properties of azobenzene-fused serotonin and support its potential as a photoswitchable ligand for controlling serotonin-receptor activity.

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**Keywords:**
Multiscale Study, Photoswichable drugs, azobenzene-fused serotonin, serotonin receptor, binding affinity

# Addition Reaction Networks and Partial Ordering of Phosphorus–Sulfur Binary Compounds: A Theoretical Study

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Starting from the white phosphorus ($P_4$) tetrahedral molecule, a family of twelve phosphorus–sulphur compounds was theoretically generated through a systematic addition-reaction scheme. The construction of the reaction network followed two general rules. First, sulphur atoms were introduced exclusively through single-bond attachments between two phosphorus atoms, thereby excluding the possibility of multiple P–S bonds. Second, each successive addition was required to preserve a parent–daughter relationship between the precursor and the immediate product; consequently, the product generated at one step served as the precursor for the subsequent addition step.

These rules give rise to a directed reaction network of addition reactions that can be interpreted as a partially ordered set (poset). The twelve molecular species occupy different nodes of the corresponding reaction-network diagram, represented as a Hasse diagram.

Using the Gaussian 09 (G09) software package, several physicochemical properties of the twelve species—including total energy ($E$), HOMO–LUMO energy gap ($\Delta E_{H-L}$), corresponding $\lambda_{max}$ values, density, and topological surface area—were theoretically evaluated using the UB3LYP methodology with the 6-311++G(d,p) basis set. The calculated property values were subsequently subjected to partial ordering according to the established parent–daughter relationships, thereby generating a poset for each property.

The resulting partially ordered property sets were analysed using two complementary approaches: the poset-average method [1, 2] and the cluster-expansion approach [3-5]. Both methods provide a systematic means of evaluating and comparing the selected physicochemical properties across the twelve phosphorus–sulphur species. The results obtained from these two approaches show qualitatively good agreement with each other as well as with the corresponding numerical computational results.

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**Keywords:** Reaction Networks; Partial Ordering; Phosphorus–Sulfur Binary Compounds

# Spatially Resolved Energy Transfer in Hexagonal $Cs_4PbBr_6$ Microdisks Revealed by Single-Particle Spectroscopy

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## Abstract

We investigate energy transfer (ET) in hexagonal $Cs_4PbBr_6$ microdisk (MD)–$DiIC_{18}$ dye hybrids using ensemble and single-particle spectroscopy [1-2]. Efficient singlet ET from photoexcited MDs to surface-bound $DiIC_{18}$ is evidenced by donor photoluminescence quenching, enhanced dye emission, an ET-induced rise component in the dye lifetime, and strong donor–acceptor temporal correlation.[2] Cross-correlation spectroscopy further reveals ET-induced donor–acceptor anticorrelation, while simultaneous two-channel imaging confirms spatial colocalization of donor and acceptor emission.[2] Importantly, single-particle fluorescence-lifetime imaging reveals pronounced spatial heterogeneity in ET within individual MDs. The ET efficiency reaches ~53% at the core**,** compared with ~34% at the edge**,** corresponding to an approximately 55% enhancement at the core. This spatial variation originates primarily from preferential $DiIC_{18}$ accumulation within structural cavities in the MD core. The results demonstrate that ET in perovskite microstructures can be spatially engineered through local dye distribution and provide a powerful framework for designing perovskite–molecular hybrid systems for light harvesting, spectral downshifting, sensing, and photocatalysis.[2]

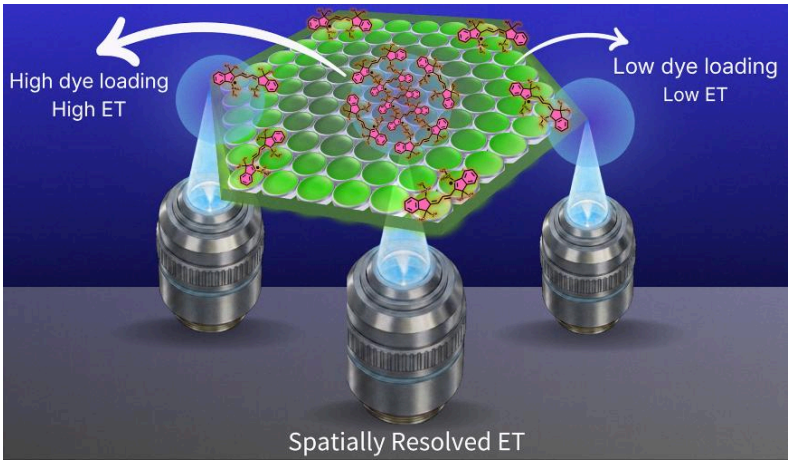



**Figure 1.** Spatially resolved ET in MD-dye composite.

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# Interfacially Engineered Liquid Crystal Microdroplets: A Robust Platform for Label-Free Optical Biosensing

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Micrometer-sized droplets of thermotropic liquid crystals (LCs) dispersed in aqueous media (i.e., LC-in-water emulsions) respond sensitively to the presence of a variety of different analytes that trigger changes in the configurations of the LC within the droplets.[1] Hereby, the analyte triggers a transition within LC droplets from a so-called 'bipolar-to-radial' configuration, visible from changes in the optical appearance of the droplets when observed using polarized optical microscopy. However, this method is not optimal as the basis of an analytical method for accurate quantification of a range of aqueous analytes for several reasons such as lack of stability of bare LC droplets, difficulty to image the droplets because of their translational and rotational mobility, and their conformational change resulting from sedimentation. In this study, we sought to develop a new strategy that involves formation of microgels decorated LC droplets by emulsifying a two- phase system wherein the organic (oil) phase is a low molecular weight LC, nematic 4-cyano-4'-pentylbiphenyl (5CB) while the aqueous phase is a dispersion of microgel particles in water. This approach provides an excellent stability to the LC emulsion droplets, the stability of which can be further tuned by incorporating charged moieties in the microgels as well as by preparing core-shell microgels. Microgels coating eliminates the droplet−surface interactions caused by sedimentation and change droplet mobility in aqueous medium, thus this approach facilitates the characterization of LC droplets using polarized light microscopy. In order to study the ability to respond to the presence of added analytes after microgels coating, we characterize the LC droplets by observing the optical appearances upon the addition of amphiphilic analytes, such as sodium dodecyl sulfate (SDS), bacterial lipopolysaccharides (LPS). The LC-in-water emulsions can be broken at temperature slightly above the volume phase transition temperature (VPTT) of the microgels that results macroscopic phase separation, thereby leading to recycling of the emulsifiers.[2] The combination of excellent emulsion stability and breaking on-demand, the responsivity of the droplets and the reusability of the emulsifier offers a complete and versatile toolbox for sustainable application of biological sensing.

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**Keywords:** Ultra-stable liquid crystal-in-water emulsions; optical detection; bacterial lipopolysaccharides

ABSTRACTS

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# Targeting *Plasmodium Falciparum* Purine Nucleoside Phosphorylase (PfPNP) with Unnatural Nucleosides: A Computational Study

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Malaria remains a major global health challenge, highlighting the need for new antimalarial agents with improved potency and selectivity [1]. Plasmodium falciparum purine nucleoside phosphorylase (PfPNP), an enzyme involved in purine metabolism, is an attractive target because its inhibition can disrupt parasite survival [2]. Here, we computationally investigated a series of designed and laboratory-synthesized ribose and deoxyribose nucleoside analogs as potential PfPNP inhibitors. Four structural series, α-ribose (Ra), β-ribose (Rb), α-deoxyribose (Da), and β-deoxyribose (Db), were evaluated using absorption, distribution, metabolism, and excretion (ADME) profiling, molecular docking, molecular dynamics (MD) simulations, molecular mechanics/generalized Born surface area (MM/GBSA) calculations and DFT mechanistic study.

The designed nucleosides showed stronger binding and greater structural stability toward PfPNP than the natural substrate inosine, with β-anomers generally exhibiting superior interactions. Several compounds also displayed improved binding compared with known PfPNP inhibitors. Density functional theory (DFT)-based calculations further showed that the selected analogs follow the same fundamental reaction pathway as inosine, but with more favorable thermodynamic or kinetic characteristics. Integrating binding, stability, and mechanistic analyses, compounds 3Ra, 7Ra, 11Ra, 6Rb, 8Rb, 11Rb, 5Db, 6Db, and 7Db emerged as promising PfPNP-targeting leads for further experimental validation and antimalarial drug development.

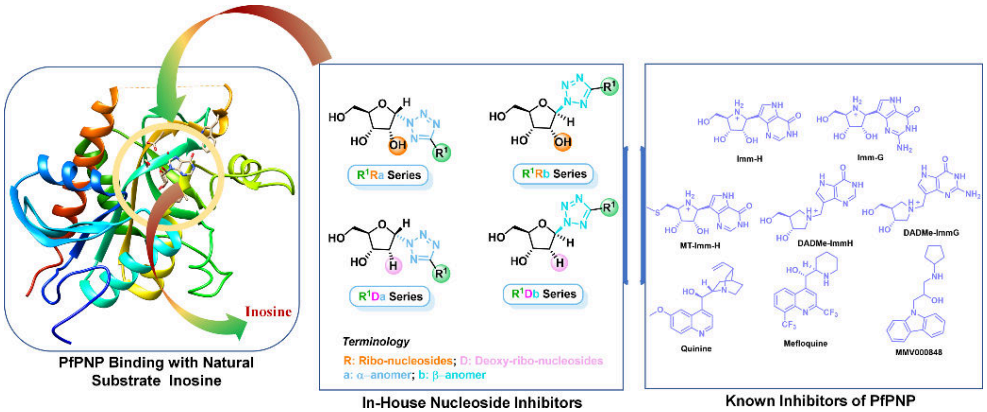



**Figure 1.** Graphical abstract of the presented work.

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**Keywords:** Malaria Drug Discovery, PfPNP, Nucleoside analogs, MD simulation, DFT.

# BSA Conjugated Carbon Nanotubes for Release of Potent Antioxidant Curcumin

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Curcumin exhibits broad anticancer potential but suffers from low solubility, rapid degradation, and limited bioavailability, restricting its therapeutic impact. To overcome these limitations, this study explores the development of bovine serum albumin (BSA)-conjugated multi-walled carbon nanotubes (MWCNTs) as an efficient nanocarrier system for curcumin adsorption,[1] controlled release, and enhanced anticancer activity.[2] BSA functionalization significantly improved the aqueous dispersibility and biocompatibility of MWCNTs, while supplying abundant surface groups capable of interacting with curcumin through hydrophobic and electrostatic forces.[2]

The resulting BSA-MWCNTs-curcumin. complexes exhibited high drug-loading capacity and a sustained, pH-responsive release pattern, with accelerated curcumin liberation under mildly acidic conditions resembling tumour microenvironments. In vitro assessments demonstrated that the nanocarrier enhanced cellular uptake and prolonged intracellular retention of curcumin, leading to increased cytotoxicity toward cancer cells compared with free curcumin. The improved performance is attributed to the synergistic effect of BSA-mediated biocompatibility and the structural features of MWCNTs that facilitate efficient adsorption and gradual release. Overall, the findings highlight BSA-conjugated MWCNTs as a promising delivery platform capable of overcoming key limitations of curcumin and offering potential advantages for targeted and sustained anticancer therapy.

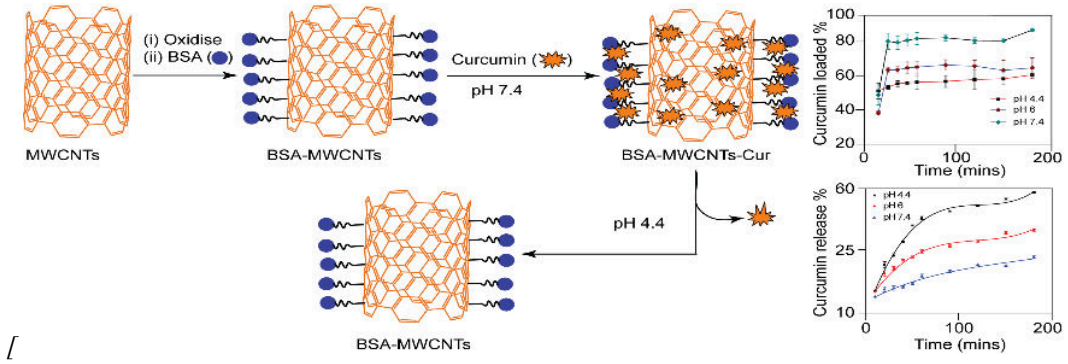



**Figure 1.** Schematic representation of proteins attached to carbon nanotubes by diimide-activated amidation.

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**Keywords:** BSA Conjugated; Curcumin Delivered; pH Sensitive Release, Anticancer

# On the origin of the structural isomerism dependent intersystem crossing : role of spin–orbit and nuclear motion assisted spin–orbit coupling

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In this work, the intersystem crossing (ISC) mechanism of three isomeric molecules, namely, methyl 2-(9H-carbazol-9-yl)benzoate (*o*-MCBA), methyl 3-(9H-carbazol-9-yl)benzoate (*m*-MCBA) and methyl 4-(9H-carbazol-9-yl)benzoate (*p*-MCBA), are investigated, with particular focus on the role of direct spin-orbit (DSO), Herzberg–Teller (HT) and spin-vibronic (SV) coupling. For *o*-MCBA and *p*-MCBA, the dominant ISC pathway between the lowest excited singlet state of charge-transfer (CT) character, $S^{o/p}_{CT_1}$, and the triplet state of mixed CT and locally-excited (LE) character, $T^{o/p}_{CT_1+LE_1}$, is found to be governed jointly by DSO and HT interactions. In contrast, for *m*-MCBA, the ISC between the lowest excited singlet, $S^{m}_{LE_1}$, and the triplet state, $T^{m}_{LE_1}$, both of LE character, proceeds primarily via HT and SV interactions. The rate constants are calculated using a time-dependent correlation function based approach. To understand the underlying ISC mechanism, we have simulated the vibrationally resolved phosphorescence spectra of the three molecules using our inhouse developed code [2]. The DSO/HT-assisted $k_{ISC}$ values for the ISC pathway between the lowest excited singlet and triplet states are found to be $0.87 \times 10^6/4.16 \times 10^6$ $s^{-1}$ for the *ortho* isomer, $1.18 \times 10^6/2.24 \times 10^6$ $s^{-1}$ for the *para* isomer, and $5.67 \times 10^3/4.02 \times 10^6$ $s^{-1}$ for the *meta* isomer. Additionally, the SV-assisted $k_{ISC}$ of *m*-MCBA is calculated to be $5.45 \times 10^6$ $s^{-1}$. Our analysis reveals that though SV coupling enhances ISC in the *meta* isomer, larger $S^{o/p}_{CT_1}$–$T^{o/p}_{CT_2+LE_2}$ and $T^{o/p}_{CT_2+LE_2}$–$T^{o/p}_{CT_1+LE_1}$ energy gaps quench SV-driven ISC in the *ortho* and *para* isomers. Collectively, this study shows that despite of sharing experimental $k_{ISC}$ values of the same order of magnitude, the three structural isomers undergo fundamentally distinct ISC mechanisms[1].

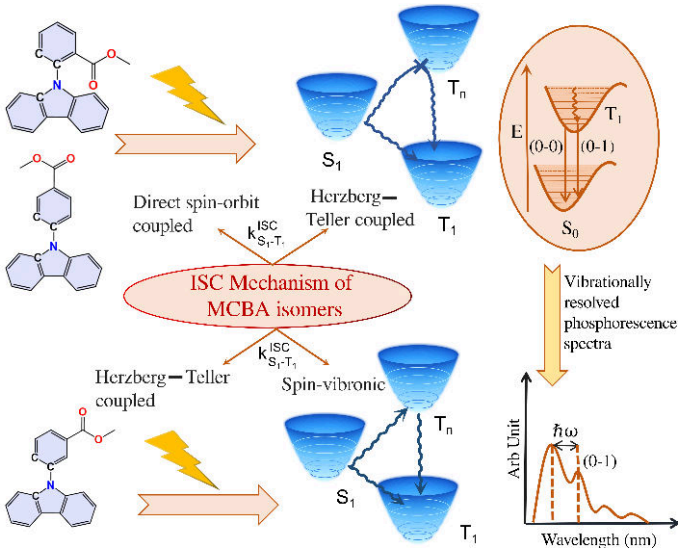



**Figure 1.** ISC mechanism of *o*-MCBA, *m*-MCBA and *p*-MCBA molecule

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**Keywords:** Inter system crossing; Spin–vibronic; Herzberg–Teller; Structural isomers

# Quantum phase transitions in time-dependent quantum mechanical scattering

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Quantum phase transitions (QPTs) [1] have served as a useful tool for characterizing qualitative changes between distinct quantum phases through the behaviour of suitable order parameters. However, their connection with the time dependent quantum mechanical processes remains quite unexplored. Establishing such connections can provide a better understanding of fundamental chemical processes especially bond making and bond breaking. This requires recasting the dynamical quantum systems in terms of appropriate thermodynamic language.

We develop a thermodynamic framework for a time-dependent quantum-mechanical scattering event by connecting it with the information-theoretic measures (generalised Rényi entropy) [2,3]. This establishes a relation between the dynamics of quantum states and thermodynamic quantities. We also construct a characteristic von Neumann entropy [4], the quantum analogue of the Shannon information entropy. Based on this description, we develop a formalism for defining an effective temperature, providing a basis for constructing the entire thermodynamic language of the scattering process. Thereafter, we use the thermodynamic description to explore the connection between scattering dynamics and quantum phase transitions (QPTs) through a system-specific order parameter.

I will briefly present our construction of the one-dimensional quantum mechanical system consisting of a Gaussian wave packet interacting with a Pöshcl-Teller potential [5], initally centered at two different positions. Additionally, I will discuss our thermodynamic formalism, including the construction of the von Neumann entropy and effective temperature along with their consequences.

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**Keywords:** quantum phase transitions; information entropies; Shannon entropy; von Neumann entropy.

# Decoding Intersystem Crossing: Molecular Design, Vibrational Control and Environmental Modulation

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Intersystem crossing (ISC) is a photophysical process which is essential for triplet-state formation, with profound implications for photocatalysis, photodynamic therapy, and optoelectronic devices. Our research combines ultrafast and steady state spectroscopy, and quantum chemical calculations to unravel how molecular structure, vibrational dynamics, and environmental factors govern ISC efficiency. Across diverse systems including aromatic carbonyls, nitroaromatic compounds, thiocarbonyls, heavy atom substituted organoboron compounds we have demonstrated that ISC is not dictated solely by static spin-orbit coupling (SOC) strength. Our findings suggest that specific bond associated vibrational modes can modulate the singlet-triplet conversion in all these compounds. For example, ISC in positional isomers in heavy-atom-substituted chromophores reveals that vibrational mixing and heavy-atom participation in key orbital transitions can influence or take precedence over SOC magnitude. Intermolecular interactions, such as hydrogen bonding, and medium viscosity further modulate ISC by reshaping nuclear motion and altering access to the singlet-triplet crossing. Collectively, these findings establish a detailed mechanistic understanding in which ISC efficiency emerges from a synergy of electronic structure, nuclear coordinates, and environmental constraints offering actionable design principles for next-generation triplet photosensitizers and photochemical systems.

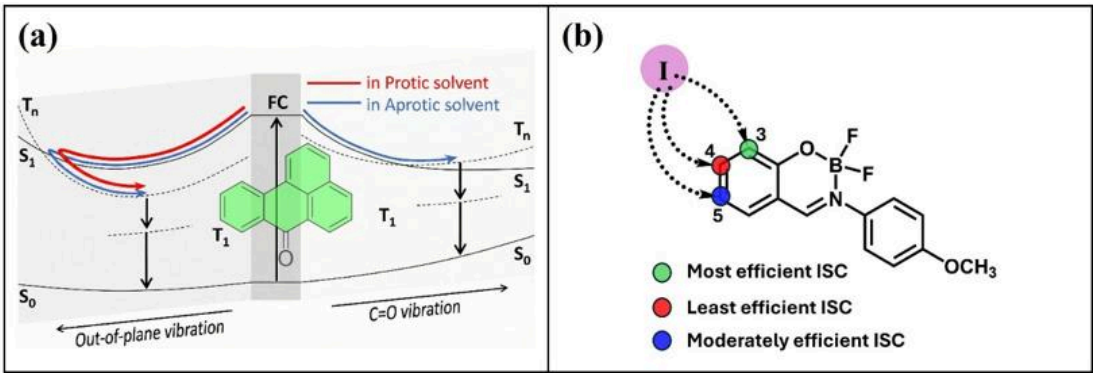



**Figure 1.** (a) Environmental/Vibrational influences of ISC in Benzanthrone; (b) Positional dependency of ISC in heavy atom substituted Salicylideneimine-Boron Compounds.

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**Keywords:** Intersystem crossing (ISC), Ultrafast Spectroscopy, Triplets, Spin-orbit-coupling

# Rethinking Activity Descriptors for Single-Atom Iron Water Oxidation Catalysts

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Due to growing demand for energy and global environmental crises, there is an urgent need to develop green and sustainable solutions to produce clean fuel and chemicals, which replace fossil fuels and reduce carbon dioxide emissions. In this regard, electrochemical water oxidation reactions play a significant role in sustainable energy storage and production. Single-atom catalysts (SACs) in particular have great attraction, yet the influence of metal loading and coordination environment on their stability, reactivity, and tunability remains unclear. While much experimental research has been done for better electrocatalyst design for OER, a thorough understanding of the catalysts under explicit electrochemical conditions is missing. Keeping focused in this direction, we have studied the number of anchored iron atoms from single to multiple metal atoms over the graphene surfaces to evaluate the reaction free-energy profiles. It is found that the single-atom iron catalyst exhibits the lowest overpotential, which is consistent with d-band centre and DOS calculations.[1,2] Grand-canonical-based quantum mechanical calculations are preferable to the computational hydrogen electrode method in evaluating the potential effect. A well-known Fe-NC material is a model system to build an electrochemical model for DFT calculations to understand the role of the electrochemical potential and electronic structures analysis. We have studied oxygen evolution reaction (OER) on a carbon-supported $FeN_4$ site by resolving high-spin (HS), intermediate-spin (IS), and low-spin (LS) states and comparing a bare (non-axial) structure with an axially water-ligated structure. Under constant potential condition, axial ligation stabilizes an IS state pathway with the lowest overpotential, whereas the non-axial site favors an HS route. Further electronic structure analysis like PDOS support these trends to potential-dependent Fe-3d orbital alignment and antibonding occupancy controlling O* and OOH* stabilization.[3]

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**Keywords:** Heterogeneous Catalysis; Density Functional Theory; Oxygen Evolution Reaction; Single Atom Catalyst.

# Deciphering bio-nano interfaces of AgNPs and $Ag_2$SNPs with HSA: mechanistic insights into protein-nanoparticle complexation and their effects on antibacterial activity

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Nanoparticles possess unique nanoscale properties that enable diverse biomedical applications, particularly in antimicrobial and therapeutic fields. These properties have enabled various biomedical applications, especially in antimicrobial and therapeutic fields. The biological functionality of silver nanomaterials is dependent on the interface formed between the nanoparticles and biological macromolecules. This work reports the formation of AgNPs and $Ag_2$SNPs with unique physicochemical properties and their bio-nano interfaces that modulate various biological activities. Neem extract acted as a reducing and stabilizing agent in the synthesis of AgNPs and $Ag_2$SNPs in aqueous medium at near-neutral pH values. The characterization of the nanomaterials was performed with ultraviolet-visible spectroscopy, powder X-ray diffraction, transmission electron microscopy, dynamic light scattering, and zeta potential. AgNPs were crystalline spherical nanoparticles with an average diameter of 14.73 ± 0.32 nm, while $Ag_2$SNPs had an average diameter of 5.22 ± 0.16 nm. Although the particles had the same silver-based composition, their interaction with human serum albumin (HSA) turned out to be quite different, since HSA created a corona of approximately 1.15–1.23 nm on the surface of AgNPs, while $Ag_2$SNPs created mostly 1:1 protein-nanoparticle complexes. The kinetics of HSA corona formation for the AgNPs were studied as well, leading to the rate constant of $0.879 \times 10^{-4}$ $s^{-1}$ $nm^{-1}$, indicating slow adsorption of HSA onto the particle surface [1]. From fluorescence, thermodynamics, and circular dichroism studies, the interaction was found to be moderate and spontaneous; besides, it was mainly governed by hydrophobic interactions. Notably, both the nanomaterials demonstrated high antibacterial activity against the tested bacterial strains, with their antibacterial efficiency being affected differently upon binding with HSA, which showed its functional significance [2]. Also, good cytocompatibility with HEK cells was observed for both types of nanomaterials. Together, these results offer an understanding of how nanoparticle composition, size, surface chemistry, and protein corona formation all contributes to the biological performance of biogenic silver nanoparticles.

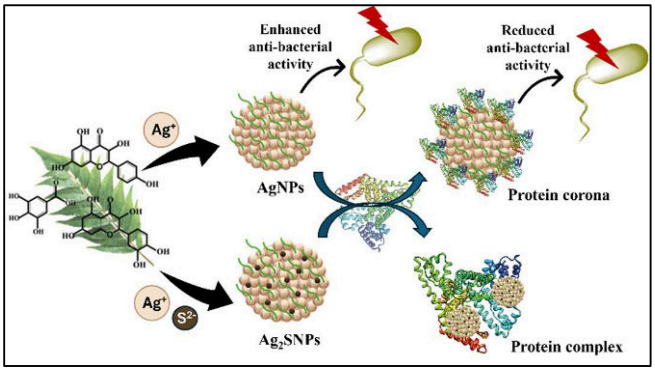



**Figure 1.** Schematic illustration of neem-mediated synthesis of AgNPs and $Ag_2$SNPs, their interaction with HSA, and the resulting influence of protein corona and complex formation on antibacterial activity.

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**Keywords:** Bio-nano interface; Corona formation kinetics; Antibacterial activity; Cytocompatibility.

# Unraveling the Dynamics of Interfacial Water at Electrified Graphene Surfaces through Theoretical Two-Dimensional Vibrational Sum-Frequency Generation Spectroscopic Study

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Understanding the interfacial behavior of water at graphene surfaces is fundamental to advances in energy storage, water desalination, biotechnology, and environmental science. Owing to its atomically smooth surface, high electrical and thermal conductivity, and chemical stability, graphene provides an ideal system for investigating molecular-level interfacial phenomena.[1] An earlier one dimensional-vibrational sum frequency generation (1D-VSFG) study showed that positive charge on graphene suppresses the intensity of the dangling (non-hydrogen-bonded) OH feature, whereas a negatively charged graphene surface enhances it, showing a charge-dependent rearrangement of the interfacial water orientation and its hydrogen-bonding networks.[2] Despite numerous studies of the structural organization and orientation of water near graphene, comparatively less attention has been paid to its dynamical behavior, particularly at electrified graphene interfaces. A recent study has shown that interfacial water exhibits slower translational and rotational dynamics near the positive electrode than that of compared with the negative electrode.[3] A molecular-level understanding of how electrode potential modulates the dynamics of interfacial water is therefore essential for understanding the behavior of electrified graphene–water interfaces. In this work, we have performed molecular dynamics (MD) simulations of a slab of 1500 water molecules between two graphene electrodes with a series of electrode potentials ranging from 0 to $\pm 1.0$ V using the constant potential method. We have calculated theoretical mid-IR two-dimensional-vibrational sum-frequency generation (2D-VSFG) spectra of interfacial water, along with their detailed layer-resolved decompositions. The transient hydrogen-bond breaking time scales of interfacial water molecules show no significant dependence on the applied electrode potential. In contrast, the characteristic time scales associated with true hydrogen-bond breaking and reformation show a pronounced dynamical slowdown at the graphene–water interface under positive applied potential. In addition, the dangling OH lifetime and the growth of the off-diagonal cross peak associated with the interconversion between hydrogen-bonded and dangling OH states differ significantly between graphene–water and air–water interfaces, despite their qualitatively similar 2D-VSFG spectral signatures.

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**Keywords:** Graphene, Graphene–Water Interface, Molecular Dynamics Simulations, 2D–VSFG, Hydrogen-bond Kinetics

# Targeting Plasmodium falciparum Calcium-Dependent Protein Kinases: Opportunities for Novel Antimalarial Therapeutics

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Malaria continues to be a major health problem worldwide, especially in tropical and subtropical areas, due to the high morbidity and mortality of *Plasmodium falciparum* and the increasing emergence of resistance against existing antimalarial drugs. Current therapies target the parasite's asexual blood stages but are largely ineffective in blocking the transmission of the parasite to mosquito vectors, thus limiting efforts to eradicate malaria. *Plasmodium falciparum* calcium-dependent protein kinases (*Pf*CDPKs), particularly *Pf*CDPK4, are among the promising molecular targets for the development of next-generation antimalarial drugs, as they are essential for parasite growth, invasion, gametogenesis and transmission. These kinases are absent in the human host, and therefore they are attractive candidates for the development of selective therapeutics with minimal toxicity to the host. The structural peculiarities, such as calcium-regulated activation, EF-hand motifs, and unique ATP-binding pockets with gatekeeper residues, offer opportunities for rational inhibitor design. Although a number of potent small-molecule inhibitors have demonstrated promising antimalarial and transmission-blocking activity, substantial gaps in knowledge still exist in their substrate specificity, signalling networks, activation mechanisms, resistance profiles, and clinical efficacy. Progress in structural biology, computational modelling, medicinal chemistry, and machine learning are expected to speed up the discovery of highly selective CDPK inhibitors and to improve the understanding of parasite signalling pathways. Therefore, *Pf*CDPKs are promising targets for developing novel transmission-blocking antimalarial drugs that may help combat drug resistance and contribute to the global efforts to eliminate malaria. [1,2]

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**Keywords:** Malaria; Calcium-dependent protein kinase (*Pf*CDPK); Kinase Inhibitors; Drug Discovery.

# Lanthanide-Doped Gold Nanocluster Assemblies Exhibiting Dopant-Directed Size Evolution, Symmetry-Controlled $Eu^{3+}$ Emission, and Selective Chemical Recognition

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The controlled doping of metal ions into nanoscale assemblies offers a powerful yet underexplored route to engineer emergent optical and chemical functionality. A central challenge lies in understanding how dopant identity simultaneously governs (i) the structural evolution of size-dependent nanocluster assemblies, (ii) the symmetry-sensitive photophysics of the dopant ion, and (iii) the collective chemical reactivity of the hybrid system. Addressing these interconnected questions is essential for rationally programming multifunctional nanoscale materials. Here, we demonstrate the controlled incorporation of $Eu^{3+}$ into zinc-mediated gold nanocluster (Zn–Au NCs) assemblies and systematically elucidate the resulting structural, photophysical, and chemical evolution. $Eu^{3+}$ doping generates a dominant emission band at 570 nm while preserving the intrinsic absorption features of the Zn–Au NCs framework, confirming electronic integration without disruption of the quantum-confined metallic core. Structurally, increasing $Eu^{3+}$ content ($Zn^{2+}$:$Eu^{3+}$ = 200:1 to 200:20) induces a systematic enlargement of the assemblies, highlighting dopant identity as a decisive factor in directing nanocluster growth. Chemically, the embedded $Eu^{3+}$ functions as a hard Lewis acidic site, enabling selective molecular recognition through hard–hard interactions and producing a ratiometric fluorescence response while maintaining stable host emission.

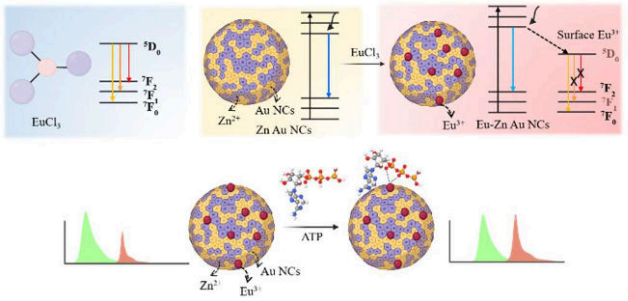



**Figure 1:** Schematic illustration depicting the photophysical evolution in $EuCl_3$, Zn Au NCs, and Eu Zn Au NCs. Illustrative depiction of ATP phosphate oxygen coordination to $Eu^{3+}$ centers in Eu–Zn–Au NCs assemblies via hard–hard Lewis acid–base interactions, resulting in enhanced $Eu^{3+}$ fluorescence while preserving the intrinsic emission of Zn–Au NCs.

**Reference:** [1]. **Ghosh S.;** Shah S-H.; Peter J.; Biswas R. K, Basu S. *J. Phys. Chem. Lett. (2026)* 17 (24): 6627–6636.

**Keywords:** Nanoclusters; defects; fluorescence; ratiometric; assembly

# Ultrafast Hole Transport via Host–Guest Binding in Perovskite Nanocrystals: Experiment and Theory

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**Abstract:** The coupling between the charge acceptors and the surfaces of nanocrystals strongly influences the charge transport properties in semiconductor nanocrystals.[1,2] A central factor governing their catalytic performance is the nature of charge transfer across the nanocrystal–molecule interface, which is insufficiently explored in formamidinium lead bromide ($FAPbBr_3$) perovskites[1]. Using three isomeric molecules of dihydroxybenzene, namely catechol (CAT), resorcinol (RES) and hydroquinone (HQ), we investigate interfacial hole transfer (HT) dynamics with distinct binding motifs that interact with $FAPbBr_3$ & $CsPbBr_3$ nanocrystals. Transient absorption spectroscopy measurements suggest that the hole transfer rate in the case of $FAPbBr_3$ to CAT is 21 ps, while it is 38 ps for HQ and no HT in the case of RES despite having favourable energetics. Complementary density functional theory (DFT) calculations and $^1H$ NMR provide atomistic insight into these interactions, revealing that both the molecular orientation of the hydroxyl groups and the A-site of the nanocrystals jointly dictate charge-transfer efficiency. CAT, with its ortho-binding geometry, highest dipole moment, and lowest ionization potential, strongly favours hole transfer by efficiently coupling to $FA^+$ sites. In contrast, RES & HQ suffer from a weak dipole moment & binding energy that fails to drive charge separation. Interestingly, the A-site $Cs^+$ ion interacts very differently with the CAT molecule, where a thermodynamically driven chelation interaction is observed. fs-TA measurements reveal that the HT rate decreases by approximately threefold (~56 ps). These findings demonstrate that interfacial binding geometry and coupling strength can outweigh thermodynamic driving force in governing charge transport dynamics.

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**Keywords**: Ultrafast hole transfer; A-site cation; dipole moment; hydrogen bonding; interfacial charge transport; binding energy; density functional theory

# Tuning Hydrogen Abstraction Reactivity of Fe(IV)=O Corrole Complexes through Local Electric Fields

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**Abstract:**

The effects of external electric fields on hydrogen abstraction (HAA) reactions mediated by metallo-porphyrins, inspired by the catalytic activity of cytochrome P450, have recently been explored both experimentally and computationally. Groves et al. reported significant catalytic activity for the oxoferryl porphyrin radical cation, [Por•+$Fe^{IV}$(O)Lax], and the hydroxoferric porphyrazine complex, [PyPz$Fe^{III}$(OH)$L_{ax}$] [1,2]. More recently, Shaik and co-workers theoretically demonstrated enhanced reactivity in charged-coronated Fe(IV)=O porphyrin systems [3].

Herein, we computationally investigate the effect of local electric fields on HAA by an Fe(IV)=O corrole complex using density functional theory. We examine the effects of field strength and orientation on the activation barrier, reaction pathway, and reactive spin state using DFT. The positively charged corrole exhibits a 3.2 kcal $mol^{-1}$ lower activation barrier than its uncharged analogue, arising from electrostatic effects of the positively charged peripheral substituents. The lower-barrier pathway proceeds on a doublet spin surface through a σ-type HAA mechanism. Analysis of the oriented local electric field further reveals that barrier lowering originates primarily from greater destabilization of the reactant relative to the transition state. Comparison with charged-coronated Fe(IV)=O porphyrins shows that the corrole system exhibits higher HAA reactivity. These findings establish oriented local electric fields as a tunable electronic parameter for modulating the reactivity of corrole-based catalysts and provide a framework for the rational design of catalysts with controllable electronic structures and reactivity.

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# Interaction Mechanism in LiH-n$NH_3BH_3$ (n=1-2) Complexes: Insights from Vibrational and Chemical Shielding Analysis

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Understanding chemical bonding is central to chemical science, as matter is organized hierarchically from molecular building blocks to higher-order assemblies. Non-covalent interactions play a crucial role in this organization by driving molecular self-assembly and can exhibit cooperative effects that enhance overall stability [1-3].

Here, the influence of LiH on $NH_3BH_3$ monomeric and dimeric complexes is investigated using DFT and MP2 methods, with DLPNO-CCSD(T) benchmarks to assess intermolecular interactions and many-body effects. QTAIM and NBO analyses indicate that stabilization is dominated by dihydrogen bonding (H···H), accompanied by strengthening of the B-N bond. Many-body energy decomposition shows that pairwise interactions account for most of the stabilization, while non-additive contributions are relatively small (~5%). Among the tested DFT methods, CAM-B3LYP-D3(BJ) and ωB97X-D3 provide a reliable description of these non-additive effects. Vibrational analysis reveals pronounced mode coupling and blue shifts in the N-H and B-N stretching modes, while chemical shielding calculations indicate that the electronic environment largely saturates upon formation of the heterodimer and reveal the anisotropic nature of the H···H interaction. Overall, LiH modulates the intermolecular interactions through coupled dihydrogen bonding, intramolecular bond strengthening, and weak many-body effects, providing molecular-level insight into hydrogen-rich systems.

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Key words: DFT, Many-body energy, cooperativity

# Enhanced Charge Transport Through Ion Networks in Highly Concentrated LiSCN-polyethylene Carbonate Solid Polymer Electrolytes

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Solid polymer electrolytes (SPEs) are promising for high energy density rechargeable Li-ion batteries (LIBs) due to high mechanical, thermal, and electrochemical stability [1]. However, low ionic conductivity ($\sigma_{dc}$) and $Li^+$-ion transference number ($t_+$) still limit the potential of SPEs. Since the discovery of polymer-in-salt (PIS) SPEs [2], highly Li-salt concentrated SPEs have provided a new avenue to improve $\sigma_{dc}$ and $t_+$ of SPEs. Challenging the preference for bulky anions due to low binding energy with $Li^+$ ion, the lithium thiocyanate-polyethylene carbonate (LiSCN-PEC) solid polymer electrolyte (SPE) demonstrates higher ionic conductivities ($3.16x10^{-5}$ S $cm^{-1}$) at polymer-in-salt concentration (100 mol%) compared to those with lithium bis(fluorosulfonyl)imide (LiFSI, $1.01x10^{-5}$ S $cm^{-1}$) and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI, $1.72x10^{-7}$ S $cm^{-1}$). Through the careful selection of PEC and LiSCN as components of SPE, the carbonyl stretching of PEC and the $SCN^-$ stretching band as vibrational reporters provide detailed structural insights into the $Li^+$ ion transport channel. Spectroscopic investigations reveal that enhanced ion aggregation alters the solvation structure around the $Li^+$ and diminishes the interaction between $Li^+$ and polymer (PEC) with increasing LiSCN concentrations, promoting faster segmental motion as a major transport mechanism. However, the transition observed from subionic to superionic behavior in the Walden plot indicates the onset of segmental motion decoupled charge transport pathway. The $SCN^-$ vibrational spectrum elucidates the evolution from a Li--SCN--Li type chain-like structure to a $Li_2$>SCN<$Li_2$ type extended ion network with increasing LiSCN concentration, revealing that the ion network provides an alternative channel for $Li^+$ ion transfer at higher concentrations, enhancing conductivity [3].

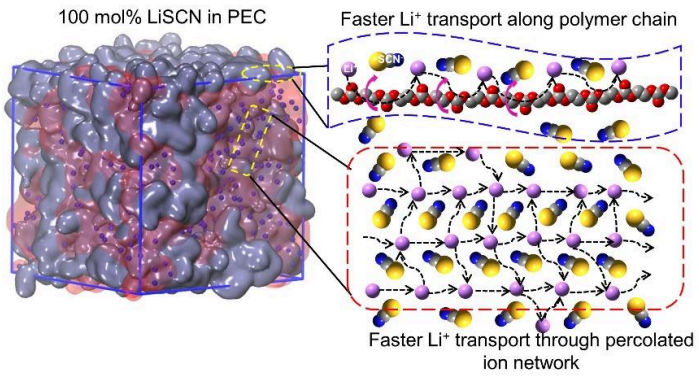



**Figure 1. The significant enhanced ion conductivity in 100 mol% LiSCN in PEC is a manifestation of combined effects arising from Li-ion transport through polymer backbone with faster polymer segmental motion and additional faster Li-ion transport through percolated ion network channel.**

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**Keywords:** enhanced ion transport; ion channels; IR spectroscopy; polymer-in-salt electrolytes; weak cation-polymer interaction

# Unravelling Magnesium Dependent Conformational Switching in Flaviviral RNA

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RNA folding into stable tertiary conformations is extremely sensitive to the concentration and the nature of surrounding counterions. Divalent metal cations strongly influence the stabilization of functionally important 3D structures and intricate tertiary interactions. Thus, ionic conditions dictate conformational heterogeneity across diverse RNA structures. In this study, we have investigated the molecular determinants underlying the distinct conformational states of Flaviviral RNA and the critical role of $Mg^{2+}$ ions in modulating its bent-to-stacked conformational switching. Flaviviruses are an emerging class of enveloped, single-stranded, positive-sense RNA viruses that include human pathogens like Dengue, Zika, Encephalitis etc. Their RNA structures exhibit complex tertiary motifs stabilized by divalent $Mg^{2+}$ ions. This study explores and compares the two distinct conformations, both in the absence and presence of crystallographic magnesium concentration by taking an X-ray crystallography-resolved structure of a functional xrRNA from Murray Valley encephalitis (MVE) virus (PDB ID: 4PQV). The MVE RNA adopts a distinct bent conformation of the P4 region, in contrast to the coaxially stacked P4–S4 architecture observed in the structurally related Zika virus RNA (PDB ID:5TPY). Notably, the MVEV structure contains 9 crystallographic $Mg^{2+}$ ions whereas Zika variant has only one, suggesting a possible role of high $Mg^{2+}$ ion concentration in stabilizing the bent conformation. To elucidate the molecular basis of this conformational difference, we performed microsecond long all atom explicit molecular dynamics simulations of the MVE RNA in the presence and absence of the crystallographic $Mg^{2+}$ ions. Remarkably, $Mg^{2+}$ ion removal induced a spontaneous transition from the bent state to a stable stacked conformation resembling the Zika architecture. This transition was accompanied by disruption of a $Mg^{2+}$-associated base triple, structural rearrangement of the P4 region and an increase in the size of the ring like architecture through which the 5' end of the RNA is sequestered. In contrast, a chelated $Mg^{2+}$-coordinated interaction was observed in the P4 region responsible for retention of the bent state, suggesting that site-specific inner-sphere ion coordination can bias the RNA conformational landscape. To further characterize the pathway of transition, we employed Well-Tempered Metadynamics, an enhanced-sampling technique that clearly identified two distinct conformational basins corresponding to the bent and stacked states. Together, these results demonstrate that $Mg^{2+}$ coordination can modulate the conformational plasticity of the MVE RNA and suggest a mechanistic basis by which crystallographic ionic conditions may regulate alternative tertiary structures of flaviviral RNA.

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**Keywords:** RNA folding; Ion induced Structural transition; Folding Free energy

# Glucose-Mediated Stabilization of Ethanol-Stressed Lipid Bilayers: Insights from Molecular Dynamics

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## Abstract

Lipid bilayers are dynamic molecular assemblies whose structural integrity can be strongly perturbed by small organic solutes such as ethanol. Previous experimental and molecular dynamics studies have shown that ethanol increases membrane fluidity, promotes lipid-chain disorder and interdigitation, and facilitates penetration into the membrane interior [1,2]. In contrast, small sugars have been shown to interact with membrane interfaces and contribute to membrane stabilization [3]. However, the molecular mechanism by which glucose counteracts ethanol-induced membrane perturbation remains insufficiently understood. Here, we employ atomistic molecular dynamics simulations to investigate the concentration-dependent interplay between ethanol and glucose in fully hydrated 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) bilayers.

Ethanol increases lateral lipid mobility, enhances acyl-chain disorder and interdigitation, reduces bilayer thickness, and promotes membrane curvature, particularly at higher ethanol concentration. Glucose preferentially accumulates near the lipid headgroups and forms hydrogen-bonding interactions with the interfacial region, consistent with its previously reported concentration-dependent regulation of DMPC structure and dynamics [4]. Increasing glucose concentration progressively reduces ethanol-induced lipid disorder, interdigitation, curvature, and lateral lipid diffusion [5]. Minimum-distance distribution analyses further indicate that glucose limits ethanol penetration toward the hydrophobic membrane interior. Umbrella-sampling calculations demonstrate that ethanol translocation across the bilayer becomes energetically less favorable in the presence of glucose, revealing a glucose-mediated increase in the resistance to ethanol penetration [5]. Overall, these results provide molecular-level insight into how interfacial glucose reorganizes lipid-solute interactions and counteracts ethanol-induced structural and dynamical perturbations, highlighting a potential mechanism for saccharide-mediated stabilization of lipid membranes under alcohol stress.

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**Keywords:** Glucose; Ethanol; DMPC lipid bilayer; Molecular dynamics; Umbrella sampling

# Enhanced Inhibition of Amyloid β Oligomerisation by a Coumarin-Chalcone Hybrid over a Coumarin Derivative

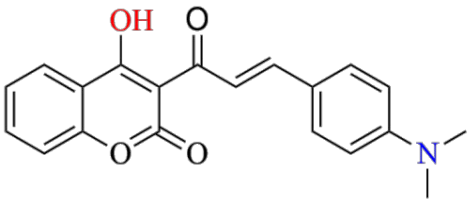
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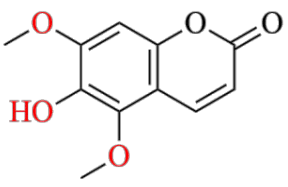
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Neurodegenerative Alzheimer's Disease (AD) is characterised by a pivotal biomarker- Amyloid Beta (Aβ) plaques found in the extracellular spaces of neurons. These insoluble Aβ plaques predominantly contain fibrillar aggregates of Aβ peptides. However, studies suggest that the intermediary oligomers are the dominant contributor of neurotoxicity in AD, rather than monomer and fibrils. Thereby, if oligomerization is inhibited at the very initiation, that may potentially disrupt the β-sheet rich structure emergence, which precedes fibril formation. AS the FDA-approved drugs provide symptomatic relief, new therapeutic strategies are in constant demand. One of effective drug scaffolds is coumarin, part of a larger class of natural benzopyrones. Coumarin and its derivatives have undergone substantial clinical studies because of their anti-cancer and anti-inflammatory activities. In our study, we have employed (i) a coumarin derivative fraxinol and (ii) a coumarin-chalcone hybrid molecule to explore the inhibitory mechanism using all-atom molecular dynamics (MD) simulation, focusing specifically on dimeric and tetrameric forms. Aβ peptides form both intra- and inter-peptide beta-sheet structures. We have implemented three force fields (ff14IDPSFF, ff99SBILDNP separately with TIP3P and TIP4P-D water), and ff14IDPSFF force field has provided approximately 30% of beta-sheet occupancy in dimeric and 15% in tetrameric forms, respectively. With the increase in the concentrations of the two drugs, we witnessed a gradual decrease in this occupancy and the removal of inter-peptide sheets. The coumarin-chalcone hybrid molecule stood out as a better scaffold, forming both electrostatic and hydrophobic interactions with the peptides, while the smaller structural framework of fraxinol provided a limited interaction interface. We predicted that in the current therapeutic strategy, rational structural hybrids have an advantageous role to play over the derivatives, because of thoughtfully engineered structural curation and focused interactive sites.




**Coumarin-chalcone hybrid molecule**




**Fraxinol**

Figure1: Structure of the Two Drugs Employed to Inhibit Aβ-Oligomerization

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**Keywords:** Alzheimer's; Aβ Oligomerization; β-sheet inhibition; Coumarin-chalcone scaffold; MD simulation

# Thermal and Light-Induced Catalysis in Pyridoxal 5′-Phosphate-Dependent Aspartate Aminotransferase

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While pyridoxal 5′-phosphate (PLP)-dependent enzymes generally operate under thermal conditions, recent experiments have shown that photoexcitation can substantially enhance their catalytic activity, although the molecular basis of this remains unclear [1]. Our previous work on the microbial aminotransferase DapC established that protein conformational dynamics and substrate-binding orientation regulate catalytic competence in PLP-dependent enzymes, highlighting the role of structural preorganization in catalysis [2]. Here, we extend this molecular-level perspective to the stereoelectronic and photochemical control of catalysis in aspartate aminotransferase (AspAT) by combining molecular dynamics (MD), quantum mechanics/molecular mechanics (QM/MM), and time-dependent density functional theory (TD-DFT) calculations employing a tuned and benchmarked range-separated double-hybrid functional. Comparison of the enzyme-bound and free external aldimine in aqueous solution shows that the AspAT active site enforces a stereoelectronically favorable Dunathan conformation and positions Lys258 to promote hyperconjugative activation of the $C_\alpha$–H bond, lowering the ground-state deprotonation barrier from 26.8 kcal/mol in water to 14.0 kcal/mol in the enzyme. Photoexcitation further modifies the reaction landscape by mixing predominantly localized $\pi\pi^*$ states with charge-transfer (CT) character involving active-site residues, particularly Lys258 and Trp142. This electronic mixing enhances spin–orbit coupling of the CT states and promotes intersystem crossing. In $T_1$, electron density shifts toward the extended LUMO and the $C_\alpha$–H antibonding region, contributing to bond weakening and lowering the deprotonation barrier to 9.8 kcal/mol in AspAT and 16.6 kcal/mol in aqueous solution. These findings reveal how active-site preorganization and specific chromophore–protein electronic interactions jointly regulate ground- and excited-state reactivity, providing a molecular framework for understanding and engineering light-driven PLP biocatalysis.

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**Keywords:** PLP, Pyridoxal 5′-phosphate; AspAT, Aspartate Aminotransferase; TD-DFT, Time-Dependent Density Functional Theory; QM/MM, Quantum Mechanics / Molecular Mechanics;

# Ligand-Specific Binding Mechanism and Dynamic Modulation of Auxin Receptor TIR1 by Structurally Diverse Auxin Analogs

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Phytohormones or plant hormones, are mostly organic molecules that play a key role in handling numerous stress signals and overall plant growth. Auxin is one of the phytohormones that is involved in the overall development of plants, regulates plant growth, and participates in resistance to abiotic stresses. In recent experimental studies, it was observed that Azelaic Acid (AZ1), 3,4-Dicholoro phenylacetic Acid (3,4-DCAA), Menthone (MNT), Geraniol (GER), Citral (Clt), 1-phenethyl-3-[3-(trifluoromethyl) phenyl] thiourea (Y21) can act as auxin analogs and show herbicidal activity. Our primary focus is understanding the mechanism of interaction between TIR1 and various auxin like herbicides. By applying molecular dynamics simulation and advanced trajectory analyses, this study will investigate binding interaction, conformational flexibility, structural stability and dynamics behavior of different ligand-bound TIR1 complexes. Our key finding is that binding with auxin, menthone and dcaa stabilize the complex by restricting the motion of TIR1 but Y21stabilizes by dynamic correlation. Comparative analyses of these interactions might provide beneficial insights into identification of eco-friendly auxin-hebicide candidates with enhanced affinity and stability.

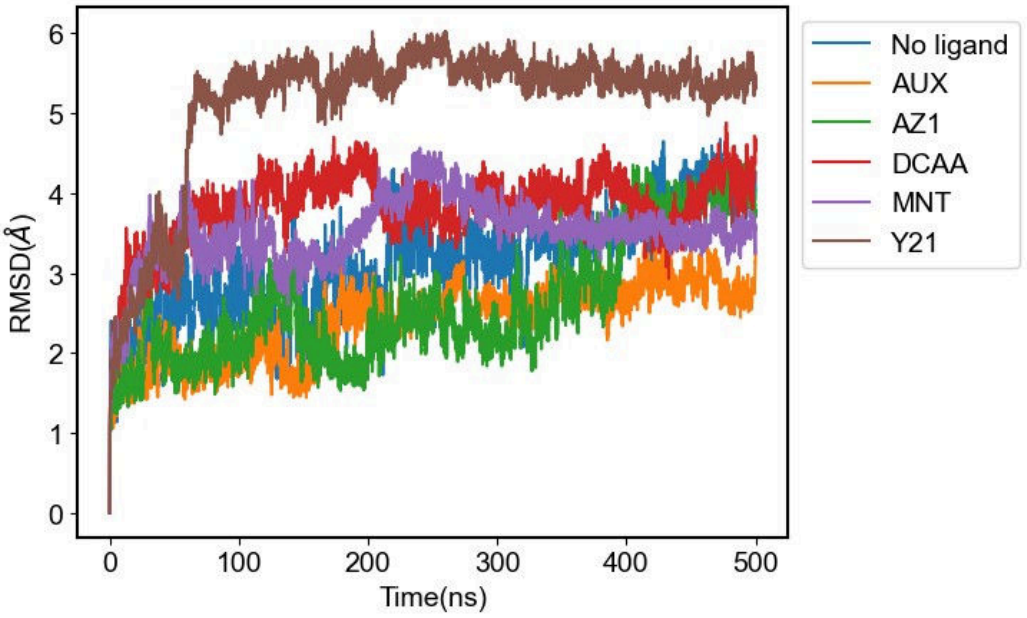



**Figure 1.** Root Mean Square Deviation Of backbone atoms of TIR1

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**Keywords:** Auxin, Herbicide, MD simulation, Dynamic modulation

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# Bile salt incorporated vesicles – Modulation of their characteristics and fluorescence probing of their microenvironment

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Different vesicular systems have been used in the past as potential Drug Delivery Systems (DDS) [1]. Liposomes were the first generation vesicles used for such applications. Due to poor stability and high cost of liposomes, alternative vesicles have been proposed over the years. Bilosomes belong to one such category. Bilosomes are biocompatible and cost effective and overcome the limitation of liposomes as DDS. Bilosomes are usually prepared from non-ionic surfactants and bile salts [2]. In the present work, Brij S2 and Brij S20 and Sodium deoxy cholate were used to prepare bilosomes. These surfactants have different *Hydrophile to Lypophile Balance* (HLB) values. After standardizing the formulations, the bilosomes were characterized using microscopy, Dynamic Light Scattering (DLS) and Small angle X-ray Scattering (SAXS). To get a better idea about the microenvironment inside these formulations, fluorescence studies were performed. A polarity probe (synthesized earlier) [3], 2-Amino-4-(1H-indol-3-yl)-4H-chromene-3-carbonitrile (AICCN) and the popular probe Nile Red (NR) were used as fluorescent probes. The results reveal interesting trends in bilosome characteristics.

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**Keywords:** Vesicles; Bile salts; AICCN

# Continuous Time Random Walk in Acetamide Deep Eutectics: Emergence of Dynamical Separation of Particles as Glass Transition is Approached

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Deep Eutectic Solvents (DESs) exhibit non-Gaussian molecular displacement distributions, reflecting their complex dynamical heterogeneity. Existing explanations primarily rely on either (i) translational jump diffusion models[1], which attribute deviations from Gaussian behavior to long-range molecular jumps and explain the breakdown of the Stokes-Einstein relation, or (ii) cage-jump mechanisms[2] based on non-local diffusion equations and quasielastic neutron scattering data, which characterize molecular caging and jumping to reveal the length and timescales of molecular displacements. However, a simple, physically interpretable theory that captures the non-Gaussian dynamics of DESs without omitting any part of the molecular motion remains unavailable. Here, we develop a Continuous Time Random Walk (CTRW) model describing the centre-of-mass motion of acetamide molecules in DESs. The model demonstrates how purely Gaussian translational displacements can collectively generate non-Gaussian dynamics through stochastic caging and waiting events. A Montroll-Weiss-type CTRW expression[3] for the self-van Hove function is fitted to Molecular Dynamics simulation data, yielding diffusion coefficients comparable to experimental values. Furthermore, while a simple CTRW model adequately describes dynamics at higher temperatures, the approach to the glass transition requires a two-population model with dynamically distinct particle groups, highlighting the increasing dynamical heterogeneity near vitrification.

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**Keywords:** Deep Eutectic Solvents; Dynamical Heterogeneity; Non-Gaussian Dynamics; Continuous Time Random Walk Model.

# OrFeaUs: Harmonic-Percussive Source Separation (HPSS)-based Feature Extraction from Molecular Dynamics Trajectories

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Interpreting molecular dynamics (MD) simulations relies heavily on systematic dimensionality reduction. Techniques such as principal component analysis (PCA) and time-lagged independent component analysis (TICA) are routinely employed to maximize the variance and the time scales of the first components, respectively. However, a crucial prerequisite for these analyses is the identification of relevant input features. Because only a small subset of coordinates drives specific biomolecular processes, it is imperative to discard uncorrelated motions and weakly correlated noise. While existing feature-selection tools effectively filter this noise using spatial community detection (e.g., MoSAIC), they often struggle to cleanly disentangle abrupt, non-linear structural transitions from continuous thermal dissipation. To address this limitation, a novel framework termed OrFeaUs (Oscillatory and Rare Event Feature Analysis Using Separation) is presented. By adapting Harmonic-Percussive Source Separation (HPSS) from acoustic signal processing, multidimensional MD trajectories are mathematically transformed into the time-frequency domain. This spectral decomposition categorizes continuous thermal basin fluctuations as "harmonic" background, while selectively isolating rare, barrier-crossing conformational changes as broadband "percussive" transients. Validated on microsecond-scale simulations of T4 Lysozyme, OrFeaUs autonomously extracts the exact temporal frames of large-scale hinge-bending transitions from high-amplitude intra-domain breathing motions. Ultimately, this framework yields collective variables with superior kinetic clarity, providing a robust, unsupervised methodology for isolating the precise geometrical features driving biomolecular function.

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**Keywords:** MD Simulation; Enhanced Sampling; Collective variables; Method development; Drug discovery

# Benchmarking Generative-AI-driven sampling of protein conformational landscapes

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Abstract

Modern protein structure prediction tools such as AlphaFold [1] have transformed our ability to identify single native fold with remarkable accuracy. Proteins are not static entities but dynamic ensembles of interconverting conformations, and these transient states are often central to function, allostery, and ligand binding. To address this, generative AI-based sampling tools such as BioEmu [2] have emerged, aiming to generate conformational ensembles directly. However, in our benchmark study we observe that BioEmu alone does not recover proper thermodynamic distributions. We therefore dig deeper into how such models might be coupled with rigorous physics-based approaches.

Using adenylate kinase (AKE), a well-characterized system with reversible open-closed transitions, we combined BioEmu-generated ensembles with short molecular dynamics (MD) trajectories and Markov State Models (MSMs). Dimensionality reduction method is applied to obtain few representative structures, that serve as seeds for multiple simulations, whose combined trajectories are used to construct a MSM. MSM analysis provides Boltzmann-weighted free-energy surfaces, enabling quantification of equilibrium populations of macrostates and substates. To assess performance, we compare our results against established enhanced-sampling methods such as umbrella sampling to benchmark the BioEmu-MSM approach in terms of efficiency, computational cost, and accuracy. This work implies that generative diffusion models, when integrated with MSMs, can accelerate exploration of protein conformational landscapes.

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**Keywords:** Protein conformational dynamics; Generative diffusion model; Molecular dynamics simulations; Adenylate kinase

# Dynamical quantum chaos in one-dimensional transverse field Ising model

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Describing chaos in the quantum regime is challenging due to the inherent position–momentum uncertainty. For several decades, considerable effort has been devoted to investigating the quantum signatures of classically chaotic systems [1]. However, a comprehensive understanding of quantum dynamics in systems governed by explicitly time-dependent Hamiltonians remains a significant challenge.

The Ising spin chain with transverse and longitudinal magnetic fields is a known system that exhibits both chaotic and integrable dynamics, depending on the choice of parameters [2]. The study of both spectral statistics and out-of-time-ordered correlators (OTOCs) supports this behaviour [3]. These calculations, however, consider only the trivial time dependence of the system. We explore the dynamical characteristics of a one-dimensional transverse-field Ising model subjected to a time-dependent oscillating magnetic field. In such a system, the tug-of-war between the nearest-neighbour spin-spin interaction and the interaction with the external magnetic field will determine the fate of the system's dynamics. The signatures of quantum chaos are probed by the Loschmidt echo (LE) [4], which indicates the absence of a chaotic nature in the dynamics. The phase-space dynamics is studied using an Ehrenfest phase-space (EPS)-like construction, considering the expectation value of the magnetization and its time derivative as equivalent to position and velocity, respectively. This enables tracking the time evolution of the spin chain in the presence of the two different kinds of interactions, along with calculations of OTOC-like quantities [5] to detect the possibility of quantum chaos.

I will present our construction of the one-dimensional transverse-field Ising model in the Hilbert space, spanned by the Pauli spin vectors. I will also discuss the primary calculations of LE with both open and periodic boundary conditions applied to the spin model. In addition, the consequences of the EPS-like construction will also be discussed.

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**Keywords:** dynamical quantum chaos; quantum Ising model; Loschmidt echo; out-of-time-ordered correlator; Ehrenfest phase space.

# A Novel Naphthofluorescein Derivative as an Antioxidant for Biodiesel: Integrated DFT, Molecular Dynamics, and Machine Learning Insights

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In this work, a new naphthofluorescein derivative (ACXB) was synthesized and characterized. The experimental characterization was performed by FT-IR, $^{1}$H-NMR, $^{13}$C-NMR, APT and LC-MS while the theoretical investigation used DFT, TD-DFT calculations, and classical molecular dynamics. The UV-Vis spectra showed absorption maxima at 305 nm, without significant solvatochromic shift. The TD-DFT calculations revealed independent nature of electronic transition to the solvent polarity. Molecular dynamics simulations in a representative biodiesel matrix composed of fatty acid methyl esters (FAMEs) indicated a persistent attractive interaction between ACXB and the organic medium, with an average interaction energy of approximately −107 kcal/mol and local organization evidenced by a radial distribution function with a maximum at 2.95 Å. Antioxidant descriptors obtained by DFT showed an N–H bond dissociation energy of 90.53 kcal/mol and an adiabatic ionization potential of 165.69 kcal/mol, suggesting that alternative mechanisms to simple hydrogen atom transfer may contribute to possible antioxidant activity. In addition, machine learning was done using XGBoost models with Morgan and MACCS fingerprints to predict the reaction rate ($K_{OH}$) against OH radicals. Together, the results identify ACXB as a naphthofluorescein derivative with high molecular compatibility with biodiesel-type matrices.

# Green's function formalism for kinetic energy density functional for atoms.

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An accurate approximation of kinetic energy density (KED) functional, is the main bottleneck in the development of orbital-free density functional theory (OF-DFT).
The total energy $E[\rho]$ contains the kinetic energy $T[\rho]$ and the potential energy $V[\rho]$ as a functional of electron density $\rho$. In contrast to $V[\rho]$, for which adequately accurate approximations exist, similar approximations are yet to be attained for $T[\rho]$ [1]. Existing kinetic energy density functionals are based on model potentials and require empirical parametrizations to obtain accurate kinetic energy of atoms . Existing KED functionals [2, 3] do not explain how $T[\rho]$ and KED are dependent on the number of electrons $(N)$, $Z$, and the spin multiplicity of the system. Also, the accuracy of the approximation involved is bench-marked against the global (integrated) value of $T[\rho]$, which fudges local details of the KED which is quintessential to produce correct shell structure. Therefore, the correct kinetic energy density which produces proper atomic shell structure remains an open problem. We have developed an exact methodology which can be used to systematically derive kinetic energy of an electronic system.
I will briefly present our formalism and it's consequences [4,5,6] I will also discuss the flagship calculations on a one-dimensional Hookian atom. These calculations successfully reproduce several salient qualitative features of atomic KEDs such as the variation of KE on number of particles. Our work shows dependence without recoursing to any asymptotic model. Furthermore, the mathematically rigorous connection between traditional Green's function and our Green's function allows for an exact recipe for the systematic development of KE.

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**Keywords:** Density functional theory; kinetic energy density functional; Green's function; orbital-free DFT

# State-specific computations of vibrational and electronic excited states

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Accurate determination of interior excited states is crucial for elucidating a range of phenomena, including core ionization, conical intersections, and high-frequency regions of vibrational spectra. Here, we present an efficient eigensolver tailored for interior vibrational states using the tree tensor network state (TTNS) ansatz, employing an inexact Lanczos method. Using this strategy, 122 states from two different spectral regions of the 12-dimensional acetonitrile molecule are accurately calculated. The algorithm also supports state following, demonstrated by targeting a Fermi resonance state of the Zundel ion. Finally, selected excited states of the higher-dimensional (33D) and more fluxional Eigen ion are computed, enabling the first full-dimensional simulation of its excited states.

For electronic problems, the coupled-cluster (CC) method works well for ground and low-lying excited states of weakly correlated systems. However, they fall short when dealing with near-degeneracies and strong correlation effects. Here, we aim to integrate two state-of-the-art techniques, CC for electronic structure and targeted eigensolvers, into a unified computational platform for state-specific calculations. We present preliminary benchmark results for the low-lying states of a few small molecules, demonstrating the viability of this approach. Ongoing work extends the method to high-lying excited states through a multireference formulation.

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**Keywords:** Vibrational state; Electronic structure; Excited state; Coupled-cluster method; Tensor network ansatz.

# Collective Reaction Dynamics during Ligand Exchange in Atomically Precise Metal Nanoclusters

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Atomically precise monolayer protected metal nanoclusters (MPCs) have gained significant attention due to their tunable physicochemical properties and their applications in diverse fields such as biomedicine, catalysis, sensing etc. Various strategies have been employed for tailoring the MPCs such as Metal doping, ligand modification etc. Among theses methods, ligand exchange stands out as versatile post synthetic tool which enables precise modulation of surface and directly influence the reactivity as well as stability of MPCs. Experimetal studies have provided valuable insights into ligand exchange processs, but understanding the detailed pathway at atomic level remains unresolved, specifically solute-solvent interations, surface dynamics during the ligand exchnage process. Computational tools such as DFT and ab initio molecular dynamics (AIMD) offer a powerful means to probe electronic structure and reaction pathways. However these methods are computationally expensive and makes it challenging to simulate realistic environments for large timescale. To address this gap, we developed and utilize machine learning potential based enhanced sampling simulations (MLIP-MD-ES) for the ligand exchange reaction in $Au_{25}(SR)_{18}$ nanocluster. In $Au_{25}(SR)_{18}$ we identify two chemically distinct, site-specific exchange pathways -*apex* and *side* routes from solution -- both exhibiting a similar free energy barrier, consistent with a facile ligand exchange reported from experimental studies. The intercluster ligand exchange proceeds *via* a stepwise substitution mechanism involving a metastable intermediate and a relatively higher free energy barrier compared to LER from solution. Our integrated MLIP-MD-ES approach employed in this study offers a generalizable computational framework for investigating complex ligand exchange mechanism by correlating electronic structure evolution, structural dynamics and free energy landscapes.

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**Keywords:** Machine Learning Potential, ligand exchange, Nanoclusters, DFT, AIMD

# Challenges in scalable excited state semiclassical dynamics

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The excited state dynamics of certain biologically relevant molecules is of great interest in our modern world, both from the perspective of energy utilization and therapeutic purposes. To theoretically simulate the dynamics, several approximations and compromises have to be made in order to make the simulation tractable. One of the most popular methods for simulating excited state dynamics is the fewest switches surface hopping (FSSH) method. Along with time dependent density functional theory providing the underlying electronic properties necessary for the propagation FSSH, this methodology predicts dynamics of excited thymine, one of the longest lived excited nucleic acids, that matches well with the spectroscopic evidences of its lifetimes. However, the FSSH simulation itself has several issues. The method effectively an heuristic, suffers from having internal inconsistencies in the excited state populations of the molecule. Furthermore, there is considerable debate surrounding the method of redistribution of the excitation energy of the molecule, which naturally affects the dynamics and finally the outcome of the molecule. Several corrections, improvements, alternate methods of propagation are being tested without losing the key feature of the FSSH method: trivial parallelization, resulting in low scaling of the method. In this presentation, we would be discussing the consequences of some of the advancements of the FSSH method on the dynamics of simple models and molecules and its effects on the excited state dynamics of thymine.

**Keywords:** nonadiabatic dynamics; excited state; electronic structure

# Quasiclassical Reaction Dynamics: Diels−Alder versus hetero-Diels−Alder Reactions

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The Diels−Alder reaction, one of the most renowned pericyclic transformations, is known for its stereospecificity proceeding through a well-defined transition state. Traditionally, it has been regarded as a concerted process leading to a single product. However, recent experimental and computational reports have shown that a single reactant can yield multiple products from the same transition state (TS). To uncover the origin of this behavior, we performed quasi-classical direct dynamics simulations coupled with density functional theory on intramolecular, intermolecular, and palladium (Pd)-catalyzed cycloaddition reactions. All the three reactions are known experimentally to produce both Diels−Alder (DA) and hetero-Diels−Alder (HDA) products. Trajectory analyses reveal evidence of post-transition state bifurcations and dynamical control of selectivity between the DA and HDA products. For the Pd-catalyzed variant, a zwitterionic entropic intermediate was identified, wherein trajectories are transiently stabilized for more than 1000 fs and 500−900 fs before collapsing to the HDA and DA products, respectively. This intermediate diverges into three distinct pathways, resulting in a pronounced trifurcation on the potential energy surface. Notably, one of them leads to the formation of a spiro-HDA product, that has not been reported previously. These findings demonstrate that reaction outcomes are not solely dictated by the statistical transition state theory but are strongly influenced by post-transition state dynamics and entropic effects, providing a deeper mechanistic understanding of how catalysts and molecular motion govern selectivity in complex cycloaddition reactions.

**Keywords:** cycloaddition reaction, [3,3]-sigmatropic rearrangement, DFT calculations, post-transition state bifurcation, entropic intermediate

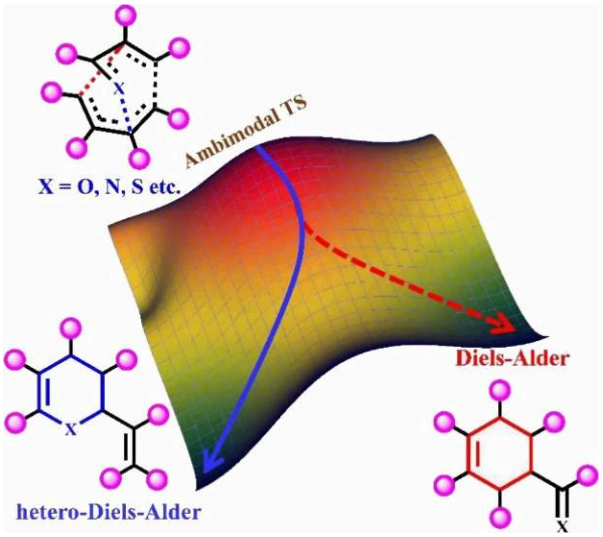



**Figure 1:** Post-Transition State Bifurcation in DA versus HDA Reactions.

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# Mapping the sgRNA-Induced Cas9 Conformational Activation Pathways Integrating Structure-Based Modeling and VAMPnet

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The CRISPR/Cas9 system constitutes a powerful genome-editing platform, in which an engineered single-guide RNA (sgRNA) programs Cas9 protein to selectively recognize and engage target DNA through sequence complementarity and introduce site-specific double stranded break. Despite its widespread application, the specific structural and functional basis by which sgRNA programs Cas9 remain incompletely understood. X-ray crystallography and electron microscopy (EM) studies have established that, apo Cas9 adopts an open, catalytically inactive conformation, whereas sgRNA binding drives the protein toward a more compact and structurally organized state, accompanied by profound domain rearrangement within REC lobe, particularly a striking rigid-body displacement of REC3 domain, from one extremity of the REC lobe to position immediately adjacent to HNH domain through an approximately 60° rotation. However, these static snapshots provide limited insight into the transition pathways and the transient intermediates underlying this large-scale rearrangement. To address this, we employed an all-atom structure-based model generated using SMOG2, in which experimentally resolved native structural information are utilized to construct the underlying Hamiltonian. By combining this structure-based model with the deep-learning approach VAMPnet, we resolved the plausible transition pathways, uncovered multiple intermediate states and identified the key residual interactions governing the apo to sgRNA-bound transition. Importantly, our analyses revealed that the statistical signature of intermediate states are already encoded within the apo-state conformational landscape, suggesting a pre-existing structural ensemble that facilitates sgRNA recognition. These findings provide molecular level perspective of Cas9 activation and may advance the rational design of Cas9 and sgRNA variants with improve specificity and reduced off-target activity.

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**Keywords:** CRISPR; Cas9; sgRNA; VAMPnet

# Investigating the nature of anion migration in halide perovskites in presence of single layer graphene

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## Abstract

The development of metal halide perovskite/perovskite heterostructures is often limited by rapid interfacial halide diffusion, which leads to the formation of mixed alloys instead of sharp and well-defined interfaces. To address this issue, Hautzinger et al. reported the use of single-layer graphene (SLG) as an ion-blocking layer between metal halide perovskite layers. [1] Their study demonstrated that SLG can effectively suppress anion diffusion in a $CsPbBr_3$/SLG/$CsPbI_3$ heterostructure, thereby significantly increasing the time required for anion migration. However, the underlying reason for this reduced anion migration remains unclear. In the present work, first-principles density functional theory calculations are used to investigate why the presence of SLG increases the timescale of anion migration across the interface. The insights obtained from this study are expected to contribute to the design and development of improved perovskite-based solar cell materials.

[1] Hautzinger et al. *J. Am. Chem. Soc.* , **2023**, 145, 2052-2057

# Variational Framework for the Calculation of Vibrational States and Thermal Properties with the Effective Harmonic Oscillator

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Predicting molecular vibrational properties accurately at both zero and finite temperatures remains challenging, particularly for large molecular systems exhibiting strong anharmonicity. In this work, we introduce a McLachlan-type variational framework for the thermal density matrix within the independent-particle model that eliminates the need for numerical integration of differential equations to determine variational parameters. The approach employs a quantum-mechanical separable ansatz for anharmonic vibrational states, together with a finite-temperature thermal density matrix to efficiently evaluate partition functions and, consequently, thermodynamic properties. First, we developed the quantum Effective Harmonic Oscillator (EHO) method, a novel variational approach for anharmonic vibrations at zero temperature [1]. The EHO method employs an effective single-particle approximation in which the variational parameters represent the centroids and widths of multidimensional Gaussian product functions, used to describe molecular vibrational wavefunctions. Benchmarking against the Vibrational Self-Consistent Field (VSCF) methods demonstrates that EHO provides comparable accuracy while substantially reducing computational cost. Next, McLachlan-type variational principle derived from the Bloch equation was developed to evaluate the finite-temperature thermal density matrix and partition function [2]. The resulting method minimizes the trace of the squared deviation between the derivatives of the exact and model density matrices. Quantum anharmonic effects are incorporated through the EHO representation, enabling efficient prediction of thermal averages over a range of temperatures. The proposed framework shows excellent agreement with thermal-VSCF and VCI methods, validating its accuracy and reliability. Most importantly, it achieves a ~98% reduction in CPU time compared with conventional approaches. These results demonstrate that the proposed variational framework offers a promising and computationally efficient alternative for studying anharmonic molecular vibrational and thermal properties at finite temperatures.

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**Keywords:** Effective Harmonic Oscillator; Bloch Equation; Potential Energy Surface; Vibrational States; Thermal Properties.

# Accelerating Selected Configuration Interaction with Restricted Boltzmann Machine

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Predicting the electronic structure of molecules where electrons are strongly correlated — as in radicals, diradicals, and extended aromatic systems — remains one of the hard problems in computational chemistry. The exact quantum mechanical treatment, full configuration interaction (FCI), scales so steeply with system size that it is intractable beyond a handful of atoms, forcing chemists to choose subsets of the electronic configurations (Slater determinants) that contribute most.

Monte Carlo configuration interaction (MCCI) addresses this by stochastically sampling and retaining only the determinants that contribute significantly to the wavefunction, but its convergence is slow, requiring many cycles of trial-and-error selection.[1] Our previous work has used artificial neural networks to learn which determinants are likely to be important and thereby speed up this search.[2] Here, we introduce restricted Boltzmann machines (RBMs) — a generative, energy-based neural network architecture — as an alternative learning engine within this active-learning framework.

Applying this RBM-guided MCCI to polyaromatic hydrocarbons, a class of molecules central to organic electronics and combustion chemistry, we show that the RBM learns the relative importance of Slater determinants more accurately and with fewer sampling cycles than prior approaches. The method successfully targets electronic states of different spin multiplicities and yields accurate singlet–triplet energy gaps, a property critical for predicting photophysical and magnetic behavior.

These results indicate that RBMs offer a more expressive and data-efficient surrogate for determinant selection than conventional neural networks, suggesting a practical path toward extending accurate multi-reference treatments of strong correlation to larger, spin-state-diverse molecular systems relevant to materials and photochemistry.

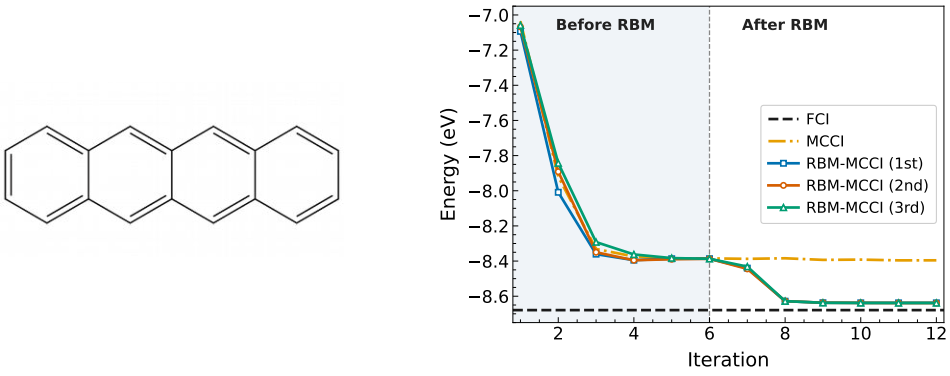



**Figure 1.** Convergence of energy along optimization of RBM-CI wavefunction for the ground state of tetracene

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**Keywords:** Strongly correlated systems; Monte Carlo configuration interaction; restricted Boltzmann machines; polyaromatic hydrocarbons; singlet–triplet gap

# From Cause to Consequence: Explainable AI-Guided Reaction Coordinate Reveals Thermodynamic and Kinetic Mechanisms of Nucleic Acid Base-Flipping

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Base flipping is a fundamental conformational transition underlying nucleic acid structural rearrangement, recognition, and function, yet the reaction coordinates governing this process across structural contexts remain poorly resolved. Here, we present an integrated framework combining enhanced-sampling molecular dynamics with a multi-evidence analysis pipeline TICA, k-means clustering, Markov state modelling, PCCA+ decomposition, and transition path theory coupled with explainable machine learning (XGBoost/SHAP) to identify the reaction coordinate that most faithfully governs base-flipping transitions.[1] Applied to HIV-1 RNA, HIV-2 RNA, and a mismatched DNA duplex, the framework reveals that flipping in each system is governed by a distinct dominant coordinate: a COM distance in some systems and a pseudo-dihedral angle in others. Within each system, the thermodynamically weighted coordinate from TICA and the causally attributed coordinate from SHAP converge on the same descriptor, indicating that both analyses detect the same underlying physical driver rather than distinct statistical artifacts. This convergence is corroborated by direct free-energy and kinetic validation: umbrella sampling in the mismatched DNA[2] using the dihedral coordinate alone resolves flipped-in and flipped-out states but fails to capture the transition barrier, whereas subsequent committor (p-fold) analysis confirms COM distance as the true reaction coordinate. This agreement across independent thermodynamic, causal, and kinetic analyses is further supported by a five-evidence statistical scheme-metastability index, block-bootstrap SHAP stability, permutation importance, SHAP dependence shape analysis, and leave-one-coordinate-out barrier sensitivity. Mean first-passage times via transition path theory further quantify flipping kinetics across systems. Together, these findings caution against assuming a universal reaction coordinate for base flipping, showing that single-evidence inference can misidentify the true barrier-controlling motion without independent thermodynamic and kinetic validation.

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# Coronene Based Two Dimensional Metal-Organic Framework with High Spin-Filtering Efficiency

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A new two dimensional periodic organometallic system, consists of amine substituted coronene moiety and different first transition series metals (Mn, Co, Cr, and Fe) has been predicted. The system has interesting electronic and magnetic properties. The ferromagnetic ground state is more stable than antiferromagnetic ground state of $C_{24}H_{12}N_8Co_2$. From the analysis of the electronic band structure it is confirmed that it is a half metallic system. Spin resolved partial density of states (PDOS) reveals that around the Fermi level the major contribution comes from 2p orbitals of carbon and nitrogen and from 3d orbitals of cobalt. The total magnetic moment of the system is found to be ~ 2 $\mu_B$. One dimensional (1-D) derivatives i.e. ribbons, which are periodic in X direction show spin semiconducting properties and the ribbons, periodic in Y direction show half metallic properties. Electronic and magnetic properties can be tuned by replacing Co by other 3d transition metals. The Fe substituted system is half metallic with magnetic moment ~ 4 $\mu_B$, while Cr substituted system is metallic with magnetic moment ~ 5.48 $\mu_B$ and Mn substituted system is spin semiconductor and possesses magnetic moment ~ 6 $\mu_B$. These systems can be used in spintronics and electronic devices and can be used as spin filtering materials.

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**Keywords**: Coronene; Semiconductor; Spin-Filtering Material; Half Metal

# Unravelling the $Mg^{2+}$-Dependent Structural Dynamics of DNA Holliday Junctions at the Single-Molecule Level

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DNA Holliday junctions (HJs) are four-stranded DNA intermediates that are critical elements in homologous recombination and DNA repair. The capacity of HJs to exist in multiple conformations is crucial for their functionality and is strongly regulated by the ionic environment.[1] In this work, we demonstrate that $Mg^{2+}$ regulates the conformational dynamics of DNA HJs as studied using single-molecule FRET (smFRET) via prism-based total internal reflection fluorescence microscopy.[2] We observe changes in smFRET distributions and transitions among conformational states in $Mg^{2+}$ dependence. Contrary to the common perception of $Mg^{2+}$ as a factor affecting only the stability of HJ structure, our results suggest that it might also influence the kinetics of conformational switching. This allows for a more sophisticated picture of how ionic strength controls the structural landscape of HJs on the level of individual molecules. The current work expands the knowledge about HJ dynamics and provides a means of studying how other factors, including DNA-processing proteins, affect recombination intermediates. Resolving the structural transitions of HJs on the level of single molecules is of importance for revealing their dynamic properties that are obscured in ensemble experiments.[3] Understanding the ion-dependent regulation of the structural transitions of HJs is critical for studying their recognition.

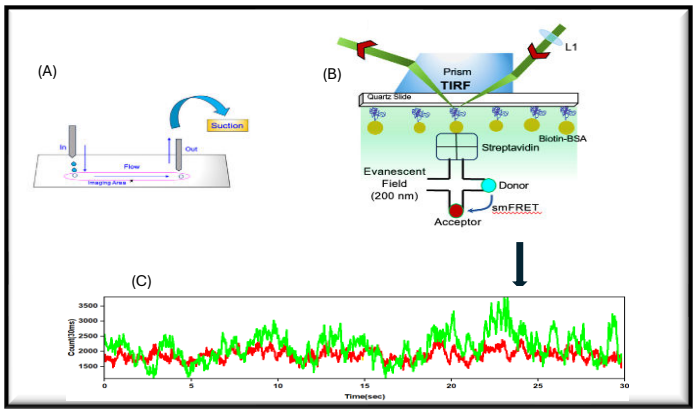



**Figure 1**. Schematic showing prism-based TIRF smFRET imaging of an immobilized DNA Holliday junction and the resulting donor–acceptor fluorescence trajectories.

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**Keywords:** smFRET, DNA Holliday Junction, Single-molecule conformational dynamics.

# Ascorbic Acid Modulates the Hydration Dynamics of Urea and Glucose: Insights from Terahertz Spectroscopy and Molecular Dynamics Simulations

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Urea (UR) and glucose (Glu) are physiologically important metabolites whose abnormal accumulation is associated with uremia and hyperglycemia, respectively. Although ascorbic acid (ASC, vitamin C) has been widely investigated for its antioxidant and protective effects under pathological conditions, the molecular basis of its interaction with UR and Glu remains poorly understood. Here, we investigate how ASC modulates the molecular association and hydration environment of UR and Glu using a combination of mid-infrared Fourier-transform infrared (MIR-FTIR) spectroscopy, terahertz time-domain spectroscopy (THz-TDS), THz-FTIR spectroscopy, and classical molecular dynamics (MD) simulations. MIR-FTIR measurements reveal characteristic vibrational shifts of UR upon ASC addition, while MD simulations identify hydrogen-bond-mediated associations between ASC and both UR and Glu, with stronger and more specific interactions predicted for UR. The simulations further show that ASC can simultaneously interact with multiple UR or Glu molecules, promoting the formation of heteromolecular clusters and restructuring their surrounding hydration environments. Consistent with the simulation results, THz-TDS measurements reveal retarded collective water dynamics in the presence of ASC, reflected in increased dielectric relaxation times, while THz-FTIR measurements demonstrate systematic changes in the hydrogen-bond stretching and librational modes of hydration water. These observations indicate substantial reorganization of the hydration environment associated with ASC–UR and ASC–Glu interactions. In addition, THz measurements of DOPC liposomes show that ASC partially attenuates the alteration of membrane-associated hydration induced by UR, suggesting a modulation of UR–membrane interfacial interactions. Collectively, these results demonstrate that ASC substantially reorganizes the aqueous and interfacial hydration environments of UR and Glu through specific intermolecular interactions, providing molecular-level insight into the physicochemical consequences of ASC association with these metabolites and a framework for further investigation of its potential physiological relevance.

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**Keywords:** Ascorbic acid, Urea, Hydration, Terahertz Spectroscopy, Molecular Dynamics (MD) Simulations

# The Fibril Tip Sets the Route, Not Just the Destination: Polymorph-Specific Kinetics of A$\beta$42 Monomer Incorporation

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Amyloid-$\beta$42 (A$\beta$42) fibrils are structurally polymorphic, and each fold presents a different template at its growing tip [1]. Whether tip architecture changes only the structure an incoming monomer eventually adopts, or also the microscopic route and kinetic cost of getting there [2], has not been tested by a matched comparison. Using adaptive molecular dynamics sampling and validated Markov state models, we followed a single A$\beta$(12–42) monomer docking at a $\nu$/U-shaped (hairpin) and an S-shaped (three-stranded) fibril tip under an identical simulation and analysis protocol. Structurally the two tips are nearly indistinguishable: both expose comparable native-like occupancy and receive the peptide through the same region in the large majority of docking events. Kinetically, however, they diverge sharply. The two folds sample their native-enriched basins to almost equal extent, yet reweighting to equilibrium leaves that basin nearly inaccessible for the $\nu$/U tip while it remains substantially populated for the S tip. Transition-path analysis shows why: the S-fold forward committor rises in graded steps toward native organisation, whereas every $\nu$/U intermediate remains too low for productive incorporation to be the likely outcome from any configuration reached. The origin traces to a single mobile strand at the $\nu$/U growth end, which remains flexible precisely while the peptide interface is still unresolved, allowing competing contacts to accumulate as misregistered kinetic traps [3] instead of consolidating. Both folds thus execute the same dock–lock mechanism, but the fibril tip – not the incoming peptide – determines whether an initial contact can be built into a committed, productive route to incorporation.

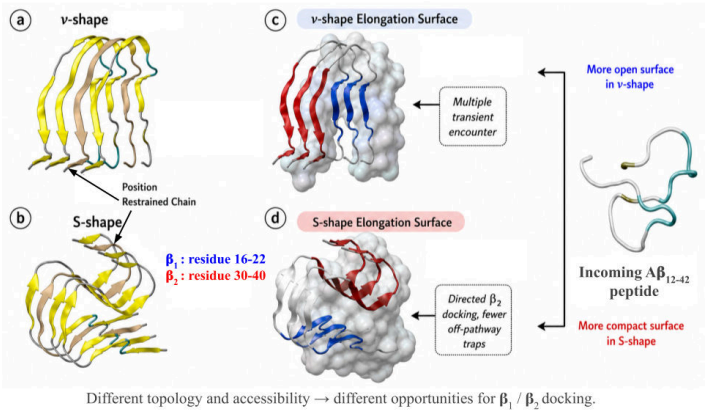



**Figure 1.** The $\nu$-shaped and S-shaped fibril elongation surfaces (a,b) expose the $\beta_1$ (residues 16–22) and $\beta_2$ (residues 30–40) segments differently (c,d): a more open surface in the $\nu$-shape permits multiple transient encounters, while the more compact S-shape surface directs $\beta_2$ docking with fewer off-pathway traps.

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**Keywords:** amyloid-$\beta$42; fibril polymorphism; Markov state models; adaptive sampling; dock–lock mechanism

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# Tailoring Herzberg-Teller Vibronic Interactions in Tetrapyrrole-Based Systems

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Nature harnesses metal tetrapyrrole frameworks in pigments such as chlorophylls and heme to enable efficient light harvesting and biochemical function [1]. In these systems, the breakdown of mirror symmetry between absorption and emission spectra is frequently observed, a feature that cannot be adequately explained within the Franck-Condon (FC) approximation alone. Instead, such deviations arise from significant Herzberg Teller (HT) vibronic coupling. A simplified FC-HT vibronic interaction model captures these effects and successfully reproduces key experimental spectral features, demonstrating that the balance and interference between FC and HT contributions are highly sensitive to chemical substitution and molecular design [2,3]. In this work, we investigate porphyrin and porphyrin-derived macrocycles with varied chemical substitutions and ligand coordination, which modulate molecular symmetry and, consequently, the electronic structure and vibronic coupling. Also, we demonstrate how solvent polarity provides an additional handle to tune the interference between FC and HT contributions in these systems. Through these systematic modifications, we aim to establish strategies to control HT interactions and, in turn, modulate excited- state dynamics. These findings provide a framework for the rational design of tetrapyrrole-based materials with tailored photophysical properties for applications in light harvesting and photonic devices.

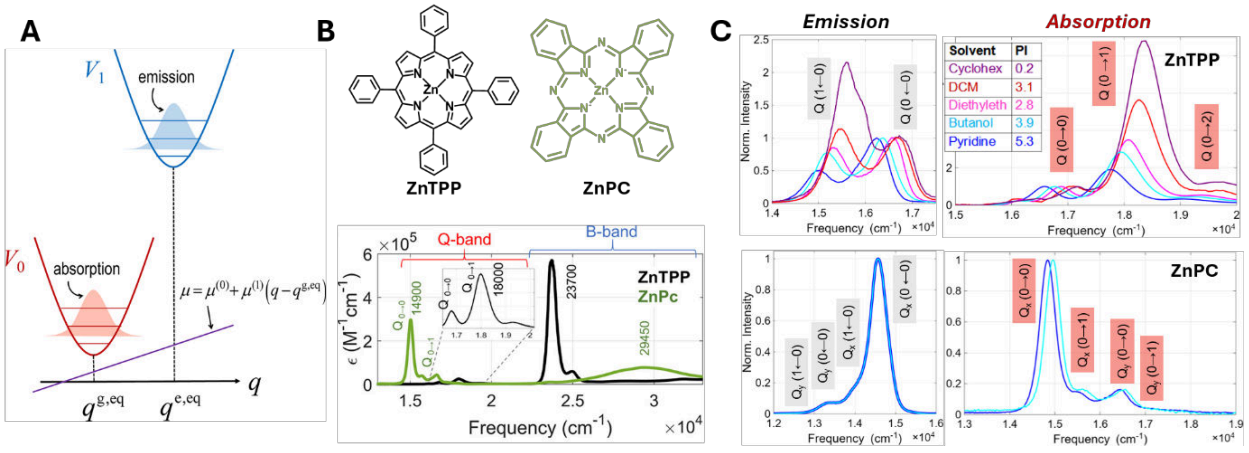



**Figure 1:** Franck-Condon and Herzberg-Teller (FC-HT) interference model, molecular structures of porphyrin systems and their solvent-dependent absorption and emission spectra.

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**Keywords:** Franck-Condon approximation, Herzberg-Teller vibronic coupling, FC-HT interference, Tetrapyrrole systems

# Structural Deviations from Ideality in Alcohol + Water Azeotropes: Molecular Scale Investigations

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Azeotropes are multicomponent liquid mixtures that boil at a constant composition under a specific temperature and pressure [1]. For example, ethanol and water forms an azeotrope at 351K, 1 atm with a composition of 0.89 mole fraction of ethanol and 0.11 mole fraction of water. They profoundly affect industrial purification as they prevent fractional distillation and alternate methods are often more complex, energy intensive and expensive. Therefore, molecular level understanding of azeotrope formation is necessary for developing affordable separation techniques. Thermodynamically, azeotropes are unique states where the excess chemical potentials of the components become identical. Yet, the process by which intermolecular organization facilitates this convergence remains unclear. Therefore, classical molecular dynamics simulations were performed to investigate the structural origins of some aqueous binary azeotropes, namely, ethanol + water and 1-propanol + water. The composition dependent centre-of-mass radial distribution functions of components showed only dilution effects, whereas higher order correlations revealed distinct structural features in azeotropes, with dominant peaks appearing at shorter distances compared to mixtures in the higher aqueous regime. In contrast, the zeotropic methanol + water system lacked such features. Since, azeotropes are also considered to be extreme manifestations of non-ideal mixture behaviour, measurements of structural excess properties are equally crucial for delineating their origins. Simulated pair correlation functions of azeotropes differed significantly from the ideal ones, with predominant peaks appearing taller and shifted at shorter distances. Later, Potential of Mean Force calculations confirmed that cross components of azeotrope undergo more favourable interactions than in the ideal mixtures. Furthermore, the characteristic structural transition at azeotropes for higher order correlations across composition range was absent for ideal mixtures, thus, providing additional evidence for favourable cross species interactions. Results suggest a crucial role of higher order correlations of components and alcohol alkyl group size in determining aqueous alcohol azeotrope formation.

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**Keywords:** Azeotropes; Molecular Dynamics Simulations; Non-Ideality; Binary Aqueous Mixtures

# Salt-Mediated Molecular Recognition of the p53 C-terminal Domain

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Intrinsically disordered proteins (IDPs) and regions (IDRs) often undergo a disorder-to-order transition upon binding to their cellular targets, yet the physical forces driving this transition—particularly the roles of long-range interactions and the ionic environment—remain debated [1]. The C-terminal domain (CTD) of the tumor suppressor p53 is a notable IDR that adopts diverse conformations depending on its binding partner. To elucidate the mechanism of coupled folding and binding, we investigated a 12-residue Short Linear Motif (SLiM) fragment of the p53 CTD as it approaches the binding cleft of the S100B protein [2]. Using all-atom molecular dynamics (MD) simulations coupled with a novel confinement setup, we explored the conformational landscape of the peptide at varying distances from the native binding surface of the partner protein in both pure water and physiological salt (0.150 M NaCl). We demonstrate a distance-dependent long-range effect where the p53 CTD, although highly disordered in pure water and in free state, spontaneously stabilizes into "bound-like" partial helical segments exclusively in the salt solution when positioned 10 Å from the native binding cleft. This stabilization effect is highly specific and vanishes at 20 Å and greater distances.

Our findings reveal that the negatively charged surface of S100B selectively organizes solvated ions at a distance, effectively projecting an electrostatic map of the binding cleft into the surrounding solvent. This creates a structured microenvironment that thermodynamically biases the p53 CTD toward its folded conformation before any direct physical contact occurs. We got similar results when taking another partner protein, Sirtuin-2, to which p53 CTD binds as beta sheet. These results highlight a synergistic mechanism between native surface topology and physiological salt, redefining the solution medium as an active, structural participant in molecular recognition.

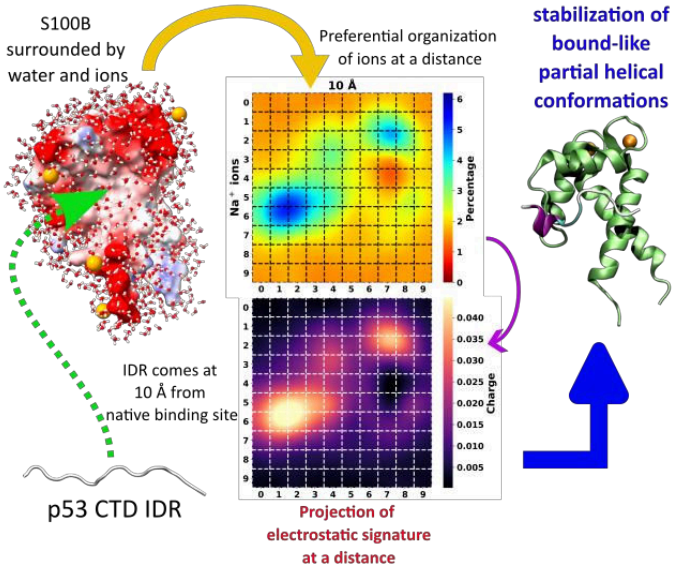



**Figure 1.** Schematic showing the preferential organization of ions near 10 Å of the native binding cleft of S100B in 0.150 M NaCl and the resultant stabilization of partial helical conformations of p53 CTD.

**References**

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**Keywords:** intrinsically disordered proteins; molecular dynamics; molecular recognition; p53 C-terminal domain; salt-mediated interactions; coupled folding and binding

# Photoswitch activity of an Acyl-hydrazone dimer: A non-adiabatic dynamics study.

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[2]*Faculty of Chemistry, Nicolaus Copernicus University in Toruń, 87-100, Poland*
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In this work, we present a non-adiabatic molecular dynamics study of an acyl-hydrazone (Ac-1) based molecule that was synthesised by Gupta et. al.[1] which shows photoswitching behaviour upon irradiation to an excited state in the presence of light. They undergo light-induced $E \rightarrow Z$ and thermal $Z \rightarrow E$ isomerization at $C = N$ bond. A dimer form of the acyl-hydrazone is considered with two different orientations of the nitrile ($C - N$) and fluorine ($F$) which are attached at the end of the phenyl rings, i.e. 'opposite' and 'same', depending on its position as shown in Figure 1. The dynamics were initiated at the $S_2$ and $S_3$ state for $EE$ and $EZ$ configurations of 'opposite' using the decoherence-corrected fewest switches surface hopping approach (DC-FSSH) and the non-adiabatic couplings between the states were computed by time-dependent Baeck-An (TD-BA) method; subsequently, conical intersections (CI) were computed for the transformation of $E \rightarrow Z$ wherein few sets of trajectories were also simulated from the CI. The full LR-TDDFT simulations and electronic structure calculations were performed at the CAM-B3LYP-D4/def2-TZVP level. The trajectories simulated hop down to $S_1$ state where the isomerization takes place and were validated by the dihedral angle changes at the $C = N$ bond at the end of the simulations.

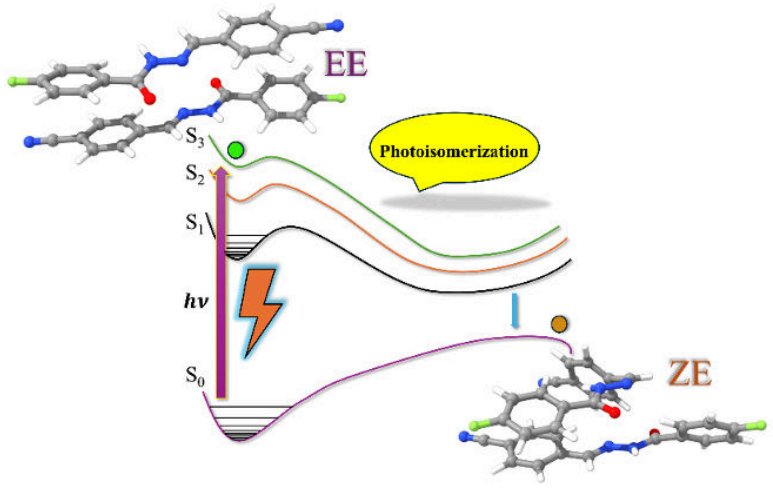



**Figure 1.** Reaction scheme considered for this study.

## References

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**Keywords:** Non-adiabatic molecular dynamics; LR-TDDFT; Conical Intersection; DC-FSSH; TD-BA

# Pepper-Mill Protein Dynamics: Decoding the Mechanism of MSPA for ssDNA Translocation

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DNA translocation through membrane-bound protein nanopores lies at the heart of both fundamental biological processes and next-generation sequencing technologies. Among these nanopores, Mycobacterium smegmatis porin A (MSPA) has emerged as a robust β -barrel protein with a narrow constriction suitable for single-molecule sensing. However, the atomic-scale mechanism by which DNA interacts and couples with the dynamic motions of the pore remains poorly understood. In this work, we combine atomistic molecular dynamics (MD) simulations with dimensionality reduction and cross-correlation analyses to elucidate the mechanism of single- stranded DNA (ssDNA) translocation through MSPA. Our results reveal a previously unrecognized "pepper mill"-like motion of MSPA during the translocation of ssDNA. This collective domain motion plays a crucial role in modulating analyte-pore interactions and influencing the dynamics of DNA passage. Furthermore, our scheme provides a generalizable and data-driven strategy for extracting mechanistic insights from large-scale biomolecular simulations. Together, these findings highlight the potential of data-driven computational strategies to guide nanopore engineering and accelerate the development of next-generation sequencing and biosensing technologies.

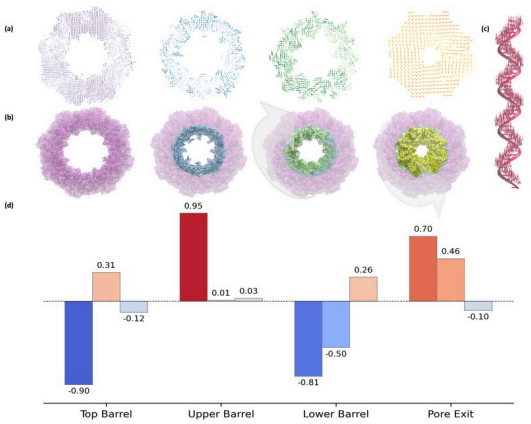



**Figure 1.** **(a) Spatial distribution of the normalized eigenvectors corresponding to the first principal component (PC1) on the xy plane, darker color represents higher magnitudes. Projection of the first principal components (PCs) for (b) the MSPA pore domains and (c) ssDNA. (d) Dynamic cross-correlation between the principal components of the MSPA pore and the first PC of ssDNA. From left to right, each bar represents the correlation of PC1, PC2, and PC3 of each protein domain with the ssDNA PC1.**

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**Keywords:** **MSPA Nanopore; PCA; Dynamic Cross-correlations; Nanopore Sequencing Technology**

# Engineering HLCT-AIE Active Molecule for Efficient Flexible Optical Waveguides: Photophysics, Mechanics, and Optoelectronic Integration

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Hybridised local and charge transfer (HLCT) emitters are gaining significant attention for organic optoelectronics due to their efficient hot-exciton utilization and tunable emission; however, merging these properties with structural flexibility remains a key challenge. Such emissions frequently suffer from reduced photoluminescence quantum yields (PLQYs) in aggregated states. In this work, we resolve this efficiency bottleneck by engineering a HLCT-AIEgen that incorporates an aggregation-induced emission (AIE)-active triphenylamine (TPA) donor, a long anthracene-π-spacer, and a moderate benzaldehyde acceptor (Figure 1a). To map out the compound's fundamental photophysics, solvent-dependent photophysical evaluations, femtosecond transient absorption spectroscopy (f-TAS), and theoretical investigations were performed. These studies confirm the formation of distinct HLCT states in low and moderately polar environments, as evidenced by unique emission profiles in toluene (TOL) and tetrahydrofuran (THF) (Figure 1b).[1]

The compound self-assembles into highly luminescent and well-ordered single crystals when grown from a hexane/ethyl acetate (2:1) mixture. Quantitative mechanical stress analyses and nanoindentation testing establish the elastic nature and structural compliance of these crystals, where a balanced supramolecular network allows for smooth layer deformation without fracturing. Leveraging this exceptional elastic flexibility and high solid-state brightness, the crystals function as robust active optical waveguides, maintaining efficient light-guiding and low-loss photonic propagation even under intense mechanical bending. This comprehensive study successfully bridges molecular architecture, crystal mechanics, and device functionality, offering a clear roadmap for the amalgamation of flexible organic single crystals into advanced integrated photonic circuits.[2]

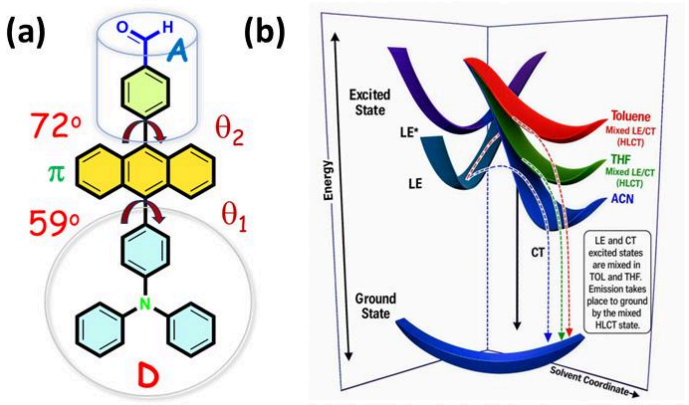



**Figure 1.** (a) The molecular structure and the dihedral angles, and (b) schematic of the probable emission mechanisms.

## References

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**Keywords:** HLCT, AIE, flexible crystal, optical waveguide

# Monitoring enzyme activity on the surface of a self-referenced near-white light emitting assembly of atomic clusters

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Sensitive and reliable detection of protease activity in complex biological environments remains a significant challenge, particularly due to signal instability, lack of internal calibration, and interference from background signals. Here, we report a self-referenced, white-light–emitting surface defect-engineered nanocluster assembly platform that enables selective and ratiometric monitoring of proteinase K activity and its inhibition. Manganese-doped, zinc-mediated gold nanocluster (Zn–Au NC) assemblies were functionalized with bovine serum albumin (BSA) to generate a tricolor emissive system comprising BSA fluorescence, nanocluster core emission, and $Mn^{2+}$-derived emission. The combined output produces near–white-light emission, providing an intrinsic internal reference for robust optical readout. Upon exposure to proteinase K, distinct and coordinated spectral changes were observed, including enhancement and blue shift of BSA emission alongside a decrease in Zn–Au NC and $Mn^{2+}$ emissions. These changes resulted in a systematic shift in chromaticity coordinates, enabling quantitative monitoring of enzyme activity through a ratiometric fluorescence response. Mechanistic studies confirmed that the optical modulation originates from proteinase K–mediated proteolytic cleavage of BSA and subsequent disruption of the nanocluster assembly, with circular dichroism providing independent validation. The platform demonstrated high selectivity toward proteinase K, effective detection of enzymatic inhibition, and reliable performance in complex biological media such as fetal bovine serum. Overall, this work[1] establishes a multifunctional, self-calibrated nanocluster-based detection strategy that translates enzymatic activity into quantifiable spectral and optical outputs. The modular design offers a versatile framework for developing enzyme-responsive probes and holds significant potential for applications in biochemical sensing, inhibitor screening, and biological diagnostics.

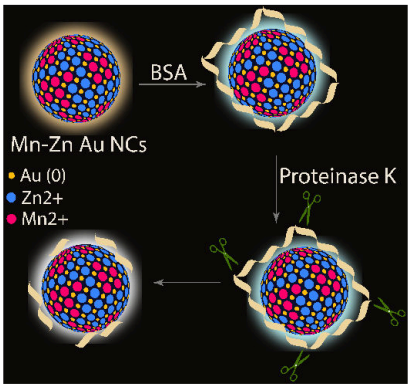



**Figure 1.** Schematic illustration depicting the use of white-light emission to monitor enzyme activity using substrate-appended, manganese-doped zinc-assembled atomic nanoclusters.

**Reference:**

1. **Sengupta,O.**; Dolai,S.; Basu, S. Monitoring enzyme activity on the surface of a self-referenced near-white light emitting assembly of atomic clusters. 2026, Under review.

**Keywords:** White light emission, fluorescence, nanoclusters, doping, enzyme activity.

# Intermediate Relaxation Timescale in Bulk Water: A Temperature-Dependent Investigation

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Water reorientation is widely described by the Laage–Hynes jump model[1], in which water molecules undergo large-amplitude angular jumps (~68°) through the breaking and formation of hydrogen bonds with different acceptors, rather than continuous diffusive rotation. Here we revisit this mechanism for both TIP5P and SPC/E water model across the temperature range 280-320K, reveals a consistent underlying mechanism for hydrogen-bond exchange. On tracking the hydrogen-bond parameters (distance, angle and acceptor-hydrogen distance) during reorientation, we identify transition states at approximately 3.3° and 38° with an acceptor–hydrogen distance cutoff of ~2.5 Å. This indicates that, on average, hydrogen-bond exchange proceeds through a distinct intermediate non-hydrogen-bonded state before the donor bonds with a new acceptor. By carefully fitting the time-correlation function of the donor O–H vector for the TIP5P model, we identified a persistent intermediate relaxation component. This relaxation time increases systematically with cooling, extending from 0.625 ps at 320 K to 1.85 ps at 280 K. Applying a wobbling-in-a-cone (WIAC) model reveals that this intermediate timescale (ranging from 1 ps to 2.6 ps for TIP5P on lowering temperature from 320K to 280K) arises from the combined contributions of a second wobbling motion and final orientational randomization. This process involves a broader angular exploration before complete randomization, expanding from ~35° to 37° for both TIP5P and SPC/E as temperature increases. Furthermore, multi-exponential analysis in the pre-jump regime effectively removes the hydrogen-bond exchange contribution from the correlation function. The resulting intermediate relaxation timescales (1 ps to 2.32 ps for TIP5P water model) closely match the WIAC analysis, successfully decoupling the orientational relaxation from hydrogen-bond exchange. This analytical approach clarifies intrinsic intermediate orientational relaxation, providing a valuable framework for understanding complex water dynamics in confined systems such as reverse micelles, hydrophobic interfaces, and spherical nanocages.

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*(#Corresponding Author: Prof. Biman Jana (e-mail: pcbj@iacs.res.in)*

**Keywords:** Hydrogen-bond exchange; Water dynamics; Extended Jump Model; Wobbling-in-a-cone

# Supramolecular assembly-driven emergent chirality with simultaneous induction and ligand inversion in atomic clusters

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Controlling chirality in nanoscale systems remains a fundamental challenge, particularly in intrinsically achiral platforms where both chiral induction and structural reconfiguration are difficult to achieve. Herein, we report a supramolecular assembly-driven strategy that enables simultaneous chiral induction, amplification, and ligand-level inversion in an initially achiral gold nanocluster system. Upon interaction with glutathione (GSH), the nanoclusters undergo hierarchical assembly into fluorescent fibrillar architectures accompanied by the emergence of strong chiroptical activity. Remarkably, the intrinsic chirality of GSH is inverted during the assembly process, revealing a unique coupling between ligand reorganization and nanocluster assembly. Spectroscopic, microscopic, and computational studies collectively indicate that ligand exchange and cooperative non-covalent interactions drive the formation of the assembled state and the associated chiroptical response. This assembly-induced reconfiguration also leads to enhanced fluorescence and amplified chiral signals. Overall, this work[1] establishes supramolecular assembly as a powerful approach for programming emergent chirality in atomically precise nanoclusters and provides a versatile framework for the design of adaptive chiral nanomaterials.

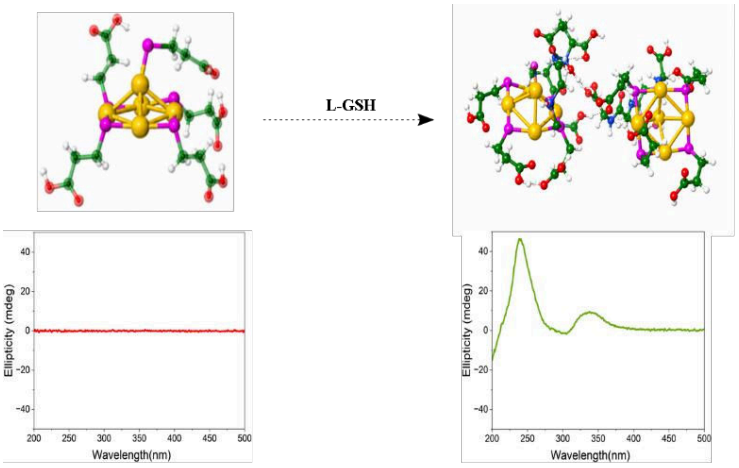



**Figure 1.** Schematic illustration of assembly mediated chiral inversion and induction.

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**Keywords:** chiral assembly; nanoclusters; chiral induction; chiral inversion; circular dichroism; fluorescence

# Determinant Sampling and Subspace Diagonalization for Strongly Correlated Molecular Systems

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**Abstract**

Accurate description of molecular electronic structure in strongly correlated regimes remains a major challenge for quantum chemistry, particularly when conventional single-reference approaches become inadequate. In this work, we investigate Sample-based Quantum Diagonalization (SQD) as a measurement-driven approach for recovering correlated molecular electronic states. Computational-basis measurements are used to identify important many-electron determinants, which are subsequently employed to construct a reduced subspace in which the molecular Hamiltonian is diagonalized classically.

We systematically investigate the relationship between determinant sampling, subspace dimension, and the quality of the recovered electronic energies. As a representative molecular test case, we study the bond dissociation of $N_2$ using the top 250, 500, 1000 and 2500 contributing determinants from the CASCI (Complete Active Space Configuration Interaction) wavefunction to construct progressively larger subspaces. The resulting dissociation curves are compared with CASCI reference calculations. Sampling configurations from the CASCI wavefunction provides an effective means of assessing the ability of the selected determinant subspace to represent the correlated electronic structure. The calculations show that the SQD approach captures the characteristic behavior of the strongly correlated dissociation regime, while the remaining energy deviation from CASCI is associated primarily with the finite dimension of the selected subspace. Increasing the number of sampled determinants systematically improves the agreement with the reference calculation.

We further investigate the sampling procedure using an LUCJ ansatz initialized from the Hartree–Fock state and executed on quantum processing units (QPUs). Similar trends are observed in the sampled configurations and reconstructed electronic energies, demonstrating the potential of combining QPU-based sampling with classical subspace diagonalization. The results highlight a promising measurement-driven framework for studying strongly correlated molecular electronic structure.

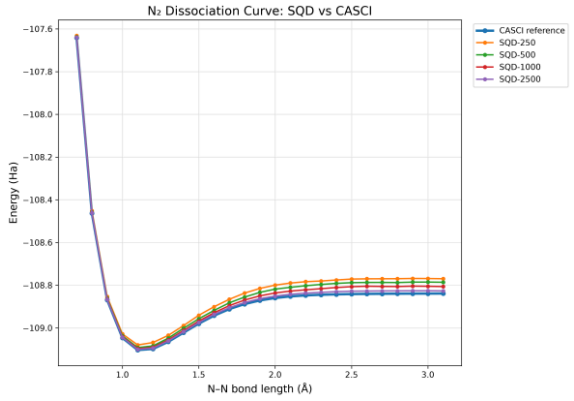



**Figure 1.** Representative $N_2$ bond-dissociation curves obtained using different numbers of sampled determinants and compared with the CASCI reference.

## References

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**Keywords:** quantum chemistry; sample-based quantum diagonalization; electronic structure; determinant sampling; strong electron correlation

# $Mg^{2+}$-Dependent Dynamics and Kinetics of a DNA Holliday Junction Studied by Single-Molecule FRET

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Holliday junctions are four-stranded intermediate DNA complexes that are formed during homologous recombination and double-stranded DNA break repair events [1,2]. The structure and conformational dynamics of the four-way (Holliday) junction are strongly dependent on the presence of different metal ions surrounding the DNA molecule, and the Junction conformation has been analysed by fluorescence resonance energy transfer (FRET) [3]. However, single-molecule fluorescence resonance energy transfer (smFRET) is an advanced and powerful optical technique that can characterize such intricate dynamic behaviours at the single-molecule level in real time, with high spatial and temporal resolution [1]. In this work, we found that single-molecule fluorescence measurements revealed a clear $Mg^{2+}$-dependent modulation of Holliday junction conformational dynamics. At low $Mg^{2+}$ concentrations, the junction displayed larger temporal fluctuations in donor–acceptor fluorescence/FRET, consistent with increased conformational exchange between different junction states. With increasing $Mg^{2+}$ concentration, the amplitude of these fluctuations progressively decreased, indicating enhanced structural stabilization of the junction. This reduction in dynamic fluctuations was accompanied by an increase in the characteristic correlation time, suggesting slower conformational transitions at higher $Mg^{2+}$ concentrations. Furthermore, the kinetics of junction rearrangement and branch migration decreased with increasing $Mg^{2+}$ concentration, consistent with a reduced population of the intermediate open state. Together, these results indicate that $Mg^{2+}$ regulates Holliday junction dynamics in a concentration-dependent manner by both stabilizing the junction structure and modulating the kinetic barriers associated with conformational transitions and branch migration.

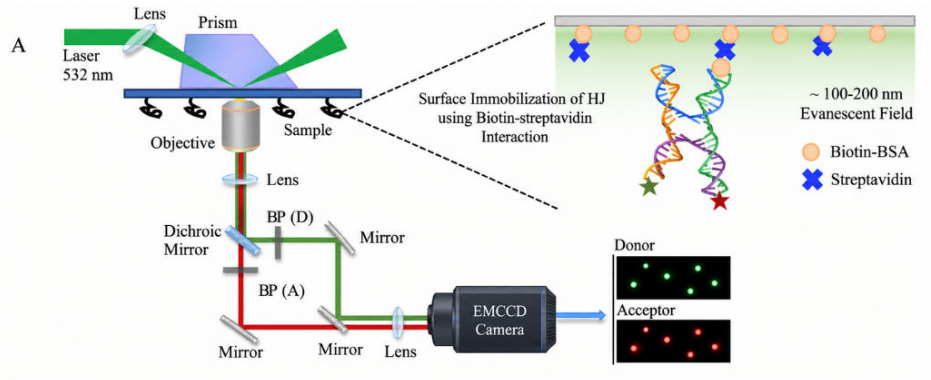



**Figure 1**. Schematic representation of prism-based total internal reflection fluorescence (FRET) microscope setup to study smFRET; a 532 nm laser beam is focused through a biconvex lens and a prism to create an evanescent field at the quartz-water interface.

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# Chemical Dynamics Simulations of Benzene-Hexachlorobenzene Complexes: Association, Ensuing Dissociation, and Comparison with Related $\pi$–$\pi$ Molecular Complexes

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Chemical dynamics simulations were employed to examine the association and ensuing dissociation behaviour of the benzene–hexachlorobenzene (Bz–HCB) complex over the temperature range of 1000–2000 K, considering impact parameters up to 10 Å. Based on intermolecular separation and lifetime, the resulting complexes were classified into two categories: short-lived and long-lived. The probability of complex formation showed a steady decline with increasing temperature, decreasing from approximately 40% at 1000 K to about 10% at 2000 K, while the corresponding lifetimes varied between 1.7 and 26.6 ps. Arrhenius analysis of the calculated association rate constants revealed that the stability of the complexes diminishes as the temperature increases. In contrast, ensuing dissociation rate constants increased with temperature for non-zero impact parameters but remained nearly unchanged for head-on collisions (b = 0.0 Å). A comparison with the benzene dimer ($Bz_2$)[1,2] and the benzene–hexafluorobenzene (Bz–HFB)[3,4] complex indicated that Bz–HCB possesses greater stability, which can be attributed to stronger $\pi$–$\pi$ interactions. Furthermore, analysis using the Rice–Ramsperger–Kassel (RRK) model suggested that complete vibrational energy randomization was not achieved in any of the systems investigated. Among them, however, the Bz–HCB complex displayed the largest effective number of vibrational degrees of freedom, reflecting stronger mode–mode coupling and repeated energy exchange between vibrational modes. This enhanced intramolecular energy redistribution contributes to its slower dissociation compared with Bz–HFB and the benzene dimer. All the calculations are done in VENUS, a chemical dynamics code.[5]

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**Keywords:** Chemical Dynamics Simulation; IVR; RRKM

# A potential gated formic acid oxidation reaction on the Rh-Cr dual-atom catalyst water interface

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The electrochemical formic acid oxidation reaction (FAOR) is crucial for the direct formic acid fuel cells (DFAFCs). Recent studies have shown that single-atom catalysts (SACs) and dual-atom catalysts (DACs) are promising catalysts in the FAOR reaction [1]. Herein, we systematically explore the dynamic, kinetic, and electronic insights into FAOR at the DAC-(Rh, Cr)/CN water interface under constant-potential conditions using a hybrid solvation model [2]. A heteronuclear Rh-Cr DAC can bypass these traditional limits by operating as a potential-gated molecular circuit. Using grand-canonical ab initio molecular dynamics (GCAIMD) at the explicit aqueous interface, we observe the reaction in real time under constant potentials of 0.2, 0.5, and 0.8 V. Our simulations reveal a remarkable division of responsibility between the two metal centers. The Cr site acts as a static anchor, spontaneously deprotonating formic acid and pinning the formate anion in a geometry that prevents the formation of carbon monoxide (CO). Meanwhile, the Rh center acts as a potential-controlled relay. The Cr center anchors the HCOO, and Rh accelerates the formate oxidation by lowering the C-H activation energy barrier. This work demonstrates that the next generation of high-efficiency electrocatalysts will not rely on a single "active" site, but on the orchestrated potential-gated synergy of dual-atom circuits that steer reaction pathways with atomic precision.

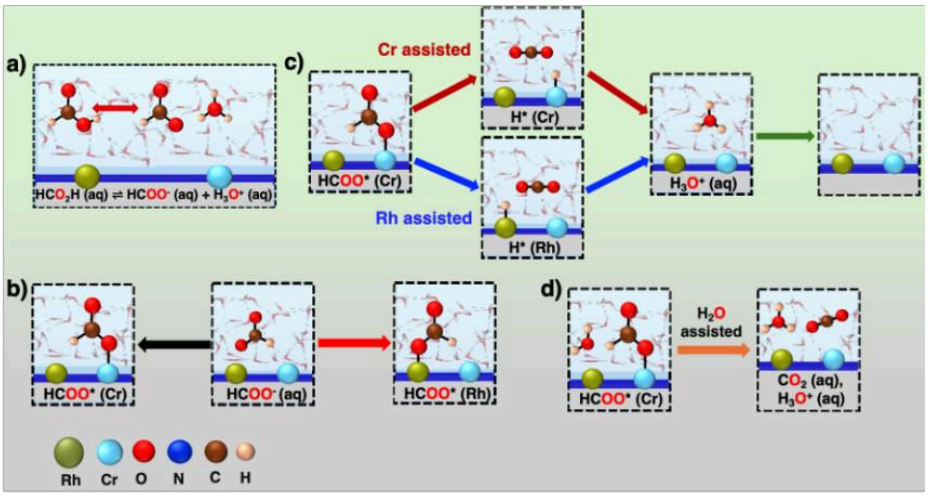



**Figure 1.** Possible reaction pathway of formic acid oxidation reaction near DAC-(Rh, Cr)/CN water interface.

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**Keywords:** Constant potential, Formic acid oxidation, c-AIMD, Dual atom catalysis, Synergistic effect.

# Unravelling the Microscopic Properties of a Globular Protein in Aqueous Deep Eutectic Solutions using Molecular Simulations

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α-Lactalbumin, the regulatory subunit of lactose synthase and a widely used model globular protein, depends on its native fold for function [1]. Deep Eutectic Solvents (DESs) have emerged as versatile, environmentally benign media whose extensive hydrogen-bonded networks make them biomimetic analogues of the crowded intracellular environment, positioning them as promising room-temperature storage media for proteins [2]. However, response of the structure, dynamics and interfacial properties of a globular protein, such as α-lactalbumin's across DES composition range — whether the medium preserves the native fold uniformly or perturbs it in a composition-dependent way — has not been resolved at the molecular level. Thus, despite its importance, the design of DES-based storage formulations largely remains empirical [3].

In this work, molecular dynamics (MD) simulations were performed to investigate the structural stability, conformational dynamics, and solvent–protein interactions of the globular protein α-lactalbumin across a range of aqueous DES compositions (0, 30, 50, 80, and 100 wt. %), spanning the dilute aqueous limit to the concentrated, cell-like regime relevant to practical storage formulations. The simulations reveal that the presence of DES modifies the hydration environment and local flexibility of the protein in a composition-dependent non-monotonic manner: protein flexibility rises from the purely aqueous system to a maximum at an intermediate DES content (~50 wt. %) and again decreases at pure DES media, reflecting a shifting balance between residual hydration and direct DES–protein contacts as the medium becomes DES rich. The preferential association of specific solvent components with the protein surface, together with the resulting residue-level changes in flexibility provide molecular-level insights into how such cell-like media influence protein conformational properties. Overall, this study demonstrates how molecular simulations can reveal the microscopic origin of protein–DES interactions and offers a composition-based framework for designing DES storage media that recreate a cell-like environment while preserving protein stability and function.

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**Keywords:** **Globular protein; Molecular simulation; Deep eutectic solvent (DES)**

# Effect of membrane composition on the structural dynamics of Amyloid Precursor Protein(APP)

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Alzheimer's disease is a neurodegenerative disorder that affects millions of people worldwide. The amyloid precursor protein is a transmembrane protein whose primary enzymatic cleavage by β-secretase produces the transmembrane C99 fragment; the latter then undergoes γ-secretase cleavage to generate amyloid-beta peptides of various lengths. The formation of amyloid-beta peptide is linked to this disease. Theoretical and experimental investigations have shown that studies on APP have mostly been done in homogeneous symmetric membranes; therefore, very limited information is available regarding the native plasma membrane. Our study provides insight into how the membrane composition affects the dynamics of APP. Here, we use molecular dynamics simulations to study C99 in symmetric and asymmetric membrane environments with different combinations of POPC, POPS, cholesterol, and sphingomyelin similar to the native plasma membrane. Our results show that membrane composition strongly modulates lipid organisation and C99 dimer structure. The radial distribution function suggests the presence of anionic lipids in the proximity of the dimer. Further addition of cholesterol and sphingomyelin increases membrane thickness and ordering of lipids. The secondary structure analysis further indicates that the change in composition affects the α-helical character of the protein. The residue-residue contact map analysis indicates more persistent and stronger interaction between the monomers as the membrane becomes more complex. Hence, in an asymmetric membrane, the strong inter-monomer contacts near the GXXXA and TVIV motifs located close to the y-secretase cleavage site may promote amyloid-beta formation. The Markov State Model analysis identified three distinct conformations of the protein based on the relative orientation of the Gly25 residue: *gly-in*, *gly-out*, and *gly-side*. Together, these findings indicate that membrane heterogeneity plays an important role in the stabilisation of the C99 protein dimer, regulating its conformation and may influence amyloid beta formation.

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**Keywords:** C99; amyloid-beta; membrane heterogeneity

# A Theoretical Investigation of the Encapsulation of Small Molecules within Coacervates of Elastin-like Polypeptides

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Elastin-like polypeptides (ELPs) are a class of bioengineered polymers that mimic the hydrophobic repeat units of tropoelastin, the precursor of elastin protein [1]. Similar to intrinsically disordered proteins (IDPs), ELPs lack a stable folded structure and exhibit sequence-encoded responsiveness to environmental stimuli such as temperature, pH, salt concentration, and the hydrophobicity of guest amino acid residues [2]. These properties enable ELPs to undergo reversible self-aggregation and phase transitions. In particular, ELPs exhibit a lower critical solution temperature (LCST), above which they undergo liquid–liquid phase separation (LLPS) and form biomolecular condensates [3,4].

In our earlier work, we employed coarse-grained molecular dynamics (CGMD) simulations with the Martini 3.0 force field to investigate the effects of temperature and polymer concentration on the coacervation of the elastin-like polypeptide sequence $(VPGIG)_{20}$ [5]. In the present study, we extend this framework to further investigate molecular processes within ELP coacervates, with a particular focus on the behaviour of small molecules inside these condensates. Specifically, we examine how the dynamics, partitioning, and diffusion of small molecules are influenced once they are encapsulated within the dense ELP phase under different thermodynamic conditions. By analysing interactions between small molecules and the coacervated ELP network, we aim to understand the mechanisms governing encapsulation efficiency, stability, and retention within the clusters. These simulations provide molecular-level insights into how sequence design and environmental parameters influence drug loading and transport within ELP condensates, thereby contributing to the development of ELP-based systems for targeted drug delivery through biomolecular condensate-mediated drug encapsulation.

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**Keywords:** Elastin-like Polypeptides; Coacervates; Encapsulation; Molecular Dynamics Simulations

# Growth of Low-Density Liquid Domains Drives Fickian, Yet Non-Gaussian Diffusion in Supercooled Water

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Using extensive all-atom molecular dynamics simulations spanning 210–320 K, we demonstrate that supercooled water exhibits a well-defined Fickian yet non-Gaussian diffusion (FnGD) regime governed by universal scaling relations. The Fickian length remains nearly temperature-independent and coincides with the first peak of the radial distribution function, while the Gaussian length grows markedly upon supercooling, producing a robust power-law coupling between the two crossover timescales, $\tau_G \propto \tau_F^{1.4}$. Rescaled displacement distributions collapse onto a universal master curve with exponentially decaying tails whose characteristic length follows $l(t) \propto t^{0.33}$. We further show that the Gaussian length marks the spatial scale at which the Stokes–Einstein relation and homogeneous Brownian transport are restored, coincident with the vanishing of translational jump diffusion. Most notably, the Gaussian length closely tracks the radius of gyration of low-density liquid (LDL) domains, establishing a direct structural origin for the FnGD regime. These results identify the growth and percolation of hydrogen-bonded LDL domains as the microscopic driver of dynamic heterogeneity in supercooled water.

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**Keywords:** Supercooled Water Anomalies; Fickian yet non-Gaussian Diffusion; LDL and HDL; Molecular Simulation.

# Vibronic Coupling Effects in the Photoelectron Spectra of $LiB_6^-$

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The present work exhibits a theoretical exploration of vibronic coupling effects in the 193 nm experimental photoelectron spectra of the $LiB_6^-$, focusing on its six lowest-lying electronic states. Based on adiabatic potential energy curves derived from *ab initio* calculations, we construct a diabatic vibronic Hamiltonian and perform nuclear dynamics by adopting TD and TI formulations of quantum mechanics, treating in adiabatic (uncoupled) and non-adiabatic (coupled) scenarios. In this study, Poisson statistics provided vibronic intensity progressions from an adiabatic perspective, and the rapid transfer of electronic population confirmed the magnitude of the non-adiabatic coupling. Our final simulated spectrum reproduces the peaks of the experimental spectra in good agreement, providing the detailed vibronic interpretation of the photoelectron spectrum of $LiB_6^-$.

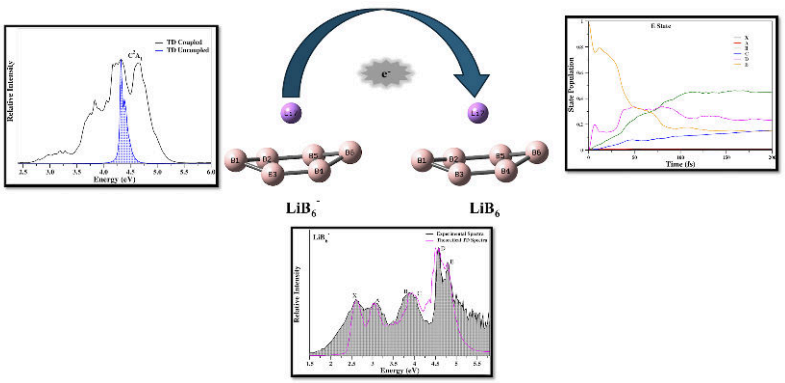



**Figure 1.** Atheoretical exploration of vibronic coupling effects in the experimental photoelectron spectra of $LiB_6^-$.

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**Keywords:** Non-adiabatic Effects; Nuclear Dynamics; Vibronic Hamiltonian; MCTDH, Photoelectron Spectroscopy

# Unravelling the role of aqueous choline chloride-polyol deep eutectic solvents in protein stability

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Protein stability is crucial for their effective usage in drug delivery, biotherapeutics, and industrial applicatins etc,. The instability of proteins often leads to degradation and loss of biological activity. In this context, Natural Deep Eutectic Solvents (NADES) have been employed as a promising alternative solvents to improve protein stability. Initially, we performed molecular dynamics simulations of aqueous DES (ADES) composed of choline chloride and three polyols - erythritol, xylitol and sorbitol, at 0, 25, 50 and 75 wt% of water to investigate structural reorganization of DES components by water. Radial distribution function (RDF) and cluster size analyses revealed that alcohol-alcohol clustering decreases with increasing water content, whereas water-water clustering shows a non-monotonic dependence, indicating the emergence of bulk like water behavior at higher hydration levels. These results highlighted the importance of tuning DES composition to control water-mediated structuring for their chemical and biological applications[1]. Subsequently, in our recent work MD simulations of lysozyme in NADES were carried out to examine the structural and dynamical properties of the system. The stable Rg, RMSD, RMSF reveals the enhanced protein compactness and stability, which was further supported by secondary structure analysis. Further, the RDFs and hydrogen bond analysis of the solvent reveal the preservation of bulk structure of the ADES components even in the presence of lysozyme[2]. Together, these results suggest that choline chloride-polyol based NADES, particularly in the presence of water provide a stabilizing environment for proteins, making them promising solvents for biotechnological and therapeutic applications.

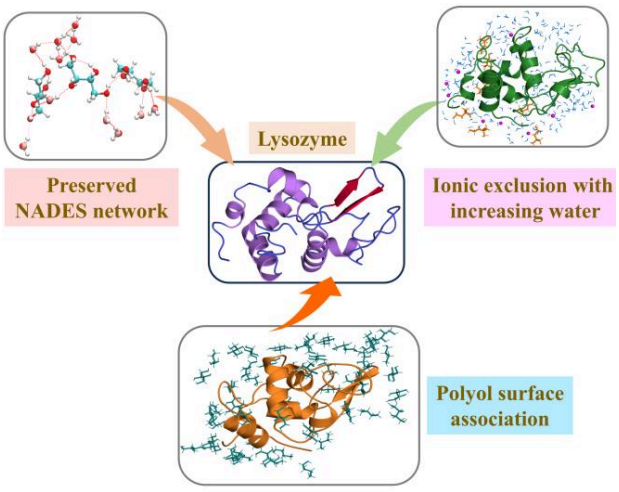



**Figure 1.** Proposed molecular mechanism underlying lysozyme stabilization in aqueous choline chloride-polyol DES

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**Keywords:** protein stability, Natural Deep Eutectic Solvents, polyol based DES, ion exclusion, hydration effects

# Emergent Mixed Crowding Effect on Protein Dimerization

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In heterogeneous cellular environment, crowders have non-specific interactions with proteins which can affect the protein-protein association or dimerization stability. Many experimental and simulation studies often incorporate homogeneous crowder environments to study crowder effects which provide limited understanding of the true *in vivo* impact. Quantifying the effect of such environment is still a formidable task. In this study, we adopt a coarse-grained model to investigate the effects of attractive lysozyme crowders on the side-by-side dimerization of GB1.[1] The effective attractive interaction between protein crowders is modeled using a Lennard–Jones-type potential, which captures the essential features of the interaction and provides qualitative agreement with experimental observations[2]. After validating the change in free energy of dimerization of single crowder environment compared to non-crowder, the study further investigates the effects of binary crowder mixtures with varying sizes and interaction potentials across different volume fractions and mixing ratios. This systematic investigation provides insight into how complex crowding environments influence the stabilization or destabilization of the dimer. In particular, it is found that smaller crowders play a superior role in overall dimer stability in binary crowder environments. Moreover, the stability of dimer formation in binary mixture of crowders arises from a delicate balance between entropy and enthalpy contributions which cannot be predicted considering the properties of individual crowders.

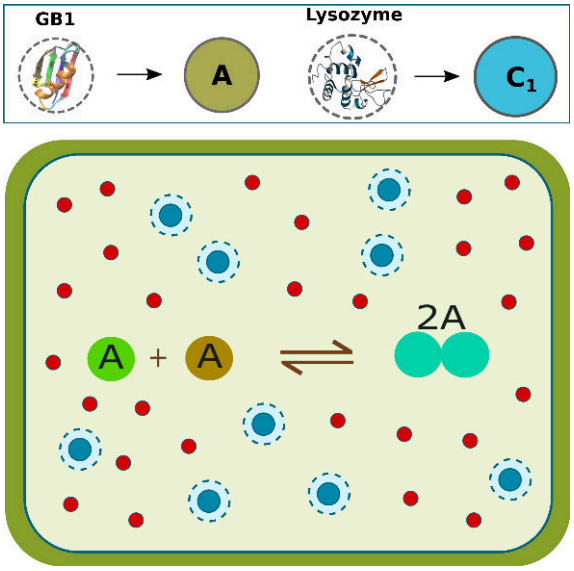



**Figure 1.** Protein dimerization in presence of mixed crowding environment.

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**Keywords:** mixed crowder; heterogeneous environment; coarse-grain models; dimerization free energy; non-specific interactions

# Anisotropic quantum beats report room temperature functional vibronic couplings in light-harvesting aggregates

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Photosynthetic bacteria and plants employ highly organized light-harvesting complexes to absorb solar energy and funnel excitons efficiently to the reaction center, where long-lived charge-separated states are formed. Cryogenic experiments and theoretical proposals have suggested a functional role of mixed vibrational-electronic (vibronic) states in the above process. Yet, at room temperature, decoherence can destroy coherent vibrational-electronic admixtures thus bringing their functionality into question. In this work, we have studied porphyrin nanotubes at room temperature as a model system for large photosynthetic aggregates. Using polarization-controlled 2DES experiments on the $Q$ band to selectively probe the $Q_x - Q_y$ coupled states, we demonstrate suppression of the prominent, but isotropic, quantum beat contributions from the observed nonlinear signal. The anisotropic quantum beats survive the polarization sequence and serve as unique reporters of functional vibronic couplings. Supporting vibronic-exciton model for the nanotube suggests that disorder may be the vital ingredient that enables electronic delocalization across overlapping vibrational-electronic manifold - vibronic couplings are not only robust to energetic disorder, but are in fact, enhanced by it across the spectral range of Q band.

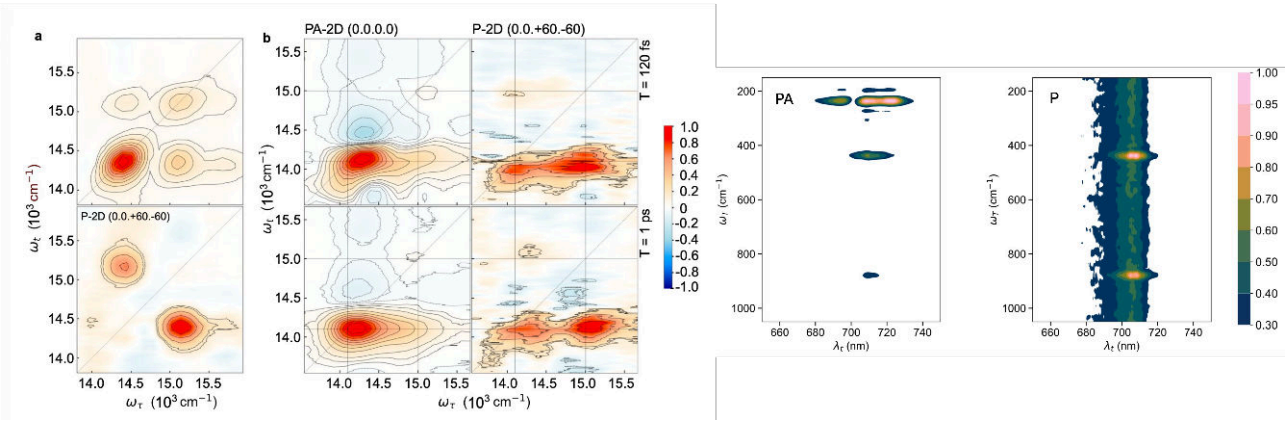



**Figure 1.** (left) Polarization controlled 2D spectra for PA and P-2D pulse sequences at T = 120 fs and 1 ps. Surviving $Q_x - Q_y$ amplitude in P-2D reveals coupled $Q_x - Q_y$ states.
(right) Quantum beat pump-probe spectra for PA (left) and P (right) pulse sequences reveals anisotropic quantum beats that survive the latter sequence, providing direct evidence of their participation in $Q_x - Q_y$ coupling.

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**Keywords:** 2DES - two-dimensional electronic spectroscopy; PA - (0.0.0.0) polarization sequence; P - (0.0.+60.-60) polarization sequence

# Engineering Heterotypic Biomolecular Condensates with Synthetic Peptides for Controlled Spatial Organization and Liquid-like Nature

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The spatial arrangement of interaction motifs within biomolecular sequences plays a central role in determining the organization, dynamics, and material properties of biomolecular condensates. Here, we investigate how sequence-encoded hydrophobicity in binary synthetic peptide systems regulates the assembly and behaviour of heterotypic condensates using coarse-grained molecular simulations. We demonstrate that differential hydrophobic interactions in binary peptides drive the emergence of distinct condensate morphologies with pronounced internal structural heterogeneity. Peptides with dominant hydrophobicity preferentially localize within the condensate core, whereas peptides with dominant charge-driven interactions accumulate near the interface in systems having significant enrichment of hydrophobic peptides, giving rise to well-defined core-surface architectures. The opposite is true in systems having profound enrichment of charge-driven peptides. As differences in hydrophobicity in peptide pairs diminish, the resulting condensate has a homogeneous mixing of the peptide pairs spatially. Spatial partitioning profoundly alters condensate dynamics, leading to differential molecular mobility between dense and dilute phases and heterogeneous relaxation behaviour within the condensed state. Our findings establish a direct link between sequence patterning, mesoscale organization, and emergent material properties, revealing sequence heterogeneity as a powerful molecular design principle for controlling condensate behaviour. By elucidating how hydrophobic and electrostatic interactions collectively govern condensate architecture and dynamics, this study provides mechanistic insights into the physicochemical principles underlying heterotypic phase separation and offers a rational framework for engineering synthetic peptide-based condensates with programmable structural, dynamic, and functional properties.

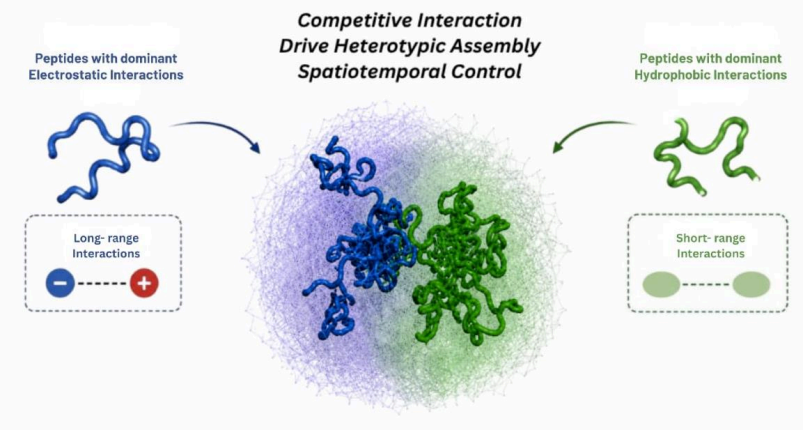



**Figure 1.** Schematic representation of Heterotypic Biomolecular Condensates with Synthetic Peptides

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**Keywords:** Biomolecular Condensates; Liquid–Liquid Phase Separation; Sequence Heterogeneity; Hydrophobic Interactions; Electrostatic Interactions.

# Molecular Insights into the Aβ-42 Tetramer Induced Disruptive Effects on a Model Phospholipid Membrane

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Formation of pores in neuronal membranes by amyloid-beta (Aβ) oligomers is believed to be the origin behind neurotoxicity in Alzheimer's disease (AD). However, despite significant efforts, high-resolution characterizations of the pore-forming Aβ oligomers from experimental studies have been hindered due to structural heterogeneity of such aggregated oligomers. Consequently, efforts have been made to characterize the aggregated oligomers that develop within a membrane environment. Attempts have been made in this study to probe the microscopic properties of the three-dimensional structure of an Aβ oligomer, specifically an Aβ-42 tetramer present in a membrane-mimicking environment. The tetramer comprises eight antiparallel β strands forming an Aβ-42 barrel. Atomistic molecular dynamics (MD) simulations at constant temperature and pressure (NPT) have been carried out on a fully hydrated liquid-crystalline lamellar phase of dipalmitoylphosphatidylcholine (DPPC) lipid bilayer with an Aβ-42 tetramer embedded into it forming a pore. The results were compared with that of a fully hydrated pure DPPC bilayer system. Based on the calculations, we have been able to successfully quantify the disruptions in the bilayer structure caused by the peptide tetramer through conformational rearrangements of the lipid hydrocarbon chains. We believe that the results presented can quantitatively provide fundamental molecular level insights on the detrimental effects of pore-forming Aβ-42 on the membrane environment, which in turn, may have important implications for Alzheimer's disease.

**Keywords:** *amyloid-beta, tetramer, dipalmitoylphosphatidylcholine (DPPC), Alzheimer's disease, β barrel*

# Quantum Dynamics and Mean Square Displacement of a Nonlinear Brownian Oscillator

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We develop a phenomenological framework for describing the statistical dynamics of dissipative quantum systems with nonlinear interactions. The analysis considers a quartic anharmonic oscillator coupled to a thermal reservoir and begins with the corresponding quantum Langevin equation. Because the resulting operator equation is nonlinear and involves higher-order moments, it is transformed into a closed equation for the second moment by employing a Gaussian closure approximation. This reduction provides a tractable description of the fluctuations while retaining the essential effects of the nonlinear interaction. To investigate the resulting dynamics, we employ a multiple-scale perturbative approach. This method separates the relevant time scales and enables the construction of an analytical solution without the secular terms that normally arise in conventional perturbation theory. The resulting expression provides a unified description of the time-dependent mean square displacement, covering both the transient regime and the long-time limit. In particular, it demonstrates how dissipation, thermal fluctuations, and the anharmonic interaction collectively influence the evolution and eventual saturation of the second moment. The analytical results also provide a possible connection between the nonlinear dynamics and experimentally measurable quantities. With recent advances in the precise measurement of particle fluctuations in optical trapping systems, the dependence of the long-time, or asymptotic, value of the second moment on the strength of the anharmonic interaction can potentially be exploited to characterize the nonlinear properties of the trapping potential. Thus, the present treatment not only provides an analytical description of dissipative quantum dynamics beyond the harmonic approximation but also suggests an experimentally accessible route for estimating the anharmonicity coefficient from equilibrium fluctuation measurements.

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**Keywords:** Quantum Langevin dynamics; Anharmonic oscillator; Mean square displacement.

# Microscopic Understanding of DNA Groove Binding by Hydrophilic and Hydrophobic Ionic Liquids

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In addition to being biologically essential macromolecules, DNAs in duplex forms also have extensive biotechnological applications[1]. DNA preservation is critical for any biotechnological use; however, long-term stability under ambient conditions remains challenging[2]. Aqueous ionic liquid (IL) solutions have evolved as excellent storage media for nucleic acid samples in recent times[3].

In this work, we have systematically investigated the interaction patterns of a series of glycinate-based ILs containing cations with varying hydrophilic and hydrophobic characteristics with duplex B-DNA using atomistic molecular dynamics (MD) simulations. The calculations revealed subtle local conformational modifications of the DNA in the presence of the ILs, though the overall DNA structure remained largely conserved. Besides, it is demonstrated that the presence of the ILs leads to nonuniform expulsion of water molecules from the minor and the major grooves of the DNA. Specifically, the propensity to exchange water molecules by the IL components is higher from the more constricted minor groove than that from the wider major groove. Furthermore, due to geometrical constraints and consequent stronger negative potential, a high degree of specificity in cation orientations and bindings has been observed within the minor groove as compared to random nonspecific cation orientations in the major groove. Importantly, an increased fraction of DNA−water hydrogen bond breaking within the minor groove in the presence of the IL cations, as compared to that in the major groove, is the microscopic origin behind such nonuniform effects on solvent properties in the two grooves. Finally, based on the findings of the present work, we believe that the degree of hydrophilicity of an IL cation can be used as an index to describe its propensity to accumulate within the DNA grooves.

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**Keywords:** duplex DNA; Ionic Liquid (IL); MD simulation.

# $CsMnBr_3$ Nanocrystals: Excitation-Dependent Photophysics and Curious Case of Carrier Dynamics from Picoseconds to Microseconds

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The photophysics of Mn-based semiconductors is commonly rationalized in terms of Mn–Mn interactions, with the interionic distance invoked as a key parameter governing radiative recombination and energy transfer. [1-2] Here, we challenge this picture through an excitation-energy-dependent investigation of purely Mn-based one-dimensional $CsMnBr_3$ metal halide nanocrystals (NCs). Contrary to the conventional expectation of excitation-independent $Mn^{2+}$ d–d emission, we uncover pronounced excitation-wavelength-dependent photoluminescence quantum yields (PLQY), reaching up to 66% under higher-energy excitation. Time-resolved optical spectroscopy further reveals excitation-dependent carrier dynamics spanning more than six orders of magnitude, from picoseconds to microseconds. This striking temporal evolution cannot be adequately described by a single $Mn^{2+}$-centered emissive pathway or solely by Mn–Mn dipole–dipole interactions. Instead, our results establish that excitation energy is one of the critical parameters for controlling the sequence of carrier relaxation, energy redistribution, and radiative recombination in $CsMnBr_3$. These findings reveal an overlooked complexity in the photophysics of Mn-based low-dimensional semiconductors and provide a new framework for understanding their PL and carrier dynamics beyond a simple Mn–Mn distance paradigm. More broadly, this work highlights excitation-selective photophysics as a powerful strategy for uncovering hidden relaxation pathways in emerging metal halide nanomaterials.

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**Keywords:** CsMnBr3 Nanocrystals, Excitation wavelength, Quantum yield, Carrier dynamics, Mn-Mn distance

# Distal residue mutations dictate substrate binding in MtbThyX

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Understanding how distal mutations disrupt enzyme function is a core challenge in drug design and resistance mapping. Here, alchemical free-energy simulations were used to quantify how second-shell mutations (Y44, Q106, Y108, and T181) alter substrate (deoxyuridine monophosphate, dUMP) binding in *Mycobacterium tuberculosis* thymidylate synthase X (MtbThyX), an essential drug target.

Substitutions like T181F and T181L drastically weaken substrate binding by more than 8 kcal/mol. Trajectories reveal that these energetic penalties stem from active-site distortion, marked by increased solvent exposure, loss of crucial electrostatic interactions, and spatial displacement of dUMP relative to the flavin adenine dinucleotide (FAD) cofactor.

These computed free-energy values rationalise experimental fitness phenotypes: mild variants (Y108F, T181S, T181A) preserve key active-site geometry, whereas deleterious mutations (T181F, Y44F, Y108S, Y44A, Q106A, T181L) collapse the necessary substrate contacts. By mapping how second-shell thermodynamics govern active-site architecture, this work provides a framework to predict mutation-driven resistance in MtbThyX and related flavin-dependent enzymes.

Keywords: second-shell residues; free energy calculations

# Dual Effect of RNA-like Polyelectrolytes on Stability and Dynamics of Biomolecular Condensates: A Tale of Competitive Short- and Long-Range Interactions

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Biomolecular condensates enable spatiotemporal organization of cellular bodies and play a central role in regulating biological rhythm. These dynamic, heterotypic assemblies often comprise proteins and RNAs in varying proportions, yet the molecular mechanisms by which RNA modulates condensate stability and dynamics remain poorly understood. Using coarse-grained molecular simulations, our study investigates RNA-like polyelectrolyte's effect on condensates formed by designed disordered peptides spanning a continuum of long and short-range interactions. By systematically varying peptide hydrophobicity and peptide–polyelectrolyte stoichiometry, we uncover a striking dual effect of RNA-like polyelectrolytes in maintaining droplet stability and dynamics. In electrostatic-dominated condensates, increasing polyelectrolyte concentration beyond an optimal level destabilizes droplets through enhanced long-range repulsions. In contrast, within hydrophobic condensates, polyelectrolytes act as multivalent interaction hubs that strengthen peptide association and enhance phase separation. These effects are reflected in condensate dynamics too, with polyelectrolytes exhibiting rapid diffusion in electrostatic-rich droplets but scaffold-like, slower dynamics in highly hydrophobic condensates. Together, our findings sum up RNA-like polyelectrolyte's effect on competing long-range electrostatic and short-range hydrophobic interactions inside condensates that tunes condensate structure, stability, and inherent molecular transport.

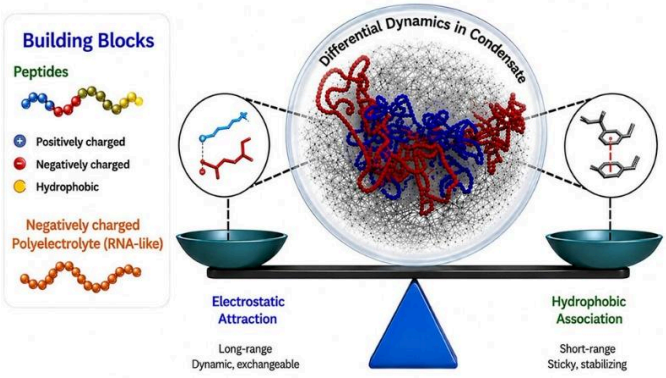



**Figure 1.** Interplay of electrostatic and hydrophobic forces governing condensates dynamics

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**Keyword:** Biomolecular condensates; Liquid-liquid phase separation; RNA-Protein interactions; Condensate dynamics.

# $Li_2O$ Vacancy-Induced Modulation of Oxygen Redox in $Li_2MnO_3$ Surfaces: A First Principles Study

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Li-rich Mn-based layered oxides (LRMOs), $xLi_2MnO_3 \cdot (1-x)LiMO_2$ ($M = Ni, Co, Mn$, etc.), are emerging high-capacity cathode materials for next-generation Li-ion batteries, owing to the additional capacity enabled by anionic redox activity [1]. In LRMO cathodes, the $Li_2MnO_3$ component is primarily responsible for the extra capacity but is also associated with poor rate performance, oxygen evolution, and layered-to-spinel phase transition. Therefore, the key challenge is to control the reversibility of oxygen redox while suppressing irreversible lattice-oxygen release. Among various modification strategies, defect engineering through controlled Li and O vacancies offers an effective approach to tune the local chemical environment and charge-compensation mechanisms without compromising the high-capacity advantage of LRMOs [2].

In this work, the influence of $Li_2O$ vacancy complexes on the oxygen redox stability of $Li_2MnO_3$ surfaces was investigated using first-principles calculations. Surface-energy calculations identified the $(131)$ and $(10\bar{1})$ facets as the most stable surfaces, with the $(131)$ surface exhibiting the lowest surface energy. The oxygen redox behaviour of the pristine and $Li_2O$-vacancy-modified surfaces was subsequently examined under different charging conditions simulated through progressive Li removal. Bader charge analysis was employed to characterize the local charge distribution of surface oxygen atoms, while electronic-structure calculations were performed to understand the effect of vacancy formation on the electronic states. Both pristine and vacancy-modified surfaces exhibited half-metallic character, with metallic states in the unoccupied spin channel. The electronic states near the Fermi level were predominantly composed of Mn and O states, indicating strong Mn–O hybridization. Further analysis of oxygen release energetics shows that the $Li_2O$ vacancy complex increases the oxygen release energy and suppresses structural changes associated with O–O dimer formation, demonstrating that surface defect engineering can stabilize lattice oxygen and promote more reversible anionic redox in Li-rich cathodes.

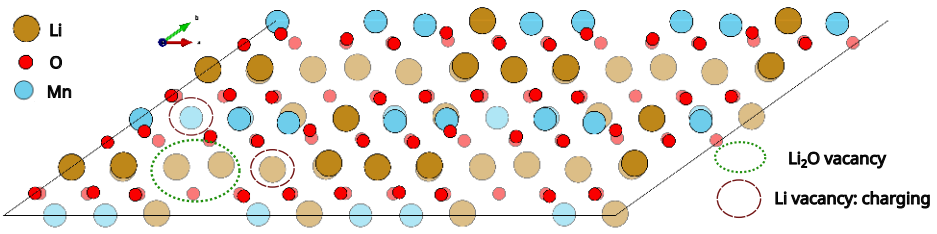



**Figure 1.** Relaxed atomic structure of the $Li_2MnO_3$ (131) surface containing a $Li_2O$ vacancy complex under 33% Li removal (charged state). The structure is viewed along the direction perpendicular to the surface.

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**Keywords:** Li-ion batteries; Cathode materials; High capacity; Anionic redox; LRMO cathodes

# Multifunctional Plasmonic Fluorescent Nanocomposites for Ultrasensitive Molecular Sensing, Antimicrobial Defense and High Resolution Bioimaging

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Plasmonic fluorescent nanocomposites (PFNs) provide a powerful platform for integrating enhanced fluorescence, ultrasensitive molecular sensing, antimicrobial defense, and bioimaging. Here, we report a $Zn^{2+}$-mediated PFN constructed through the coordination-driven assembly of 8-hydroxyquinoline-5-sulfonic acid (HQS)-stabilized silver nanoparticles (AgNPs) with a zinc quinolate complex (ZQC) [1,2]. The integration of localized surface plasmon resonance with the emissive Zn-quinolate framework produces intense green fluorescence at 530 nm, a photoluminescence quantum yield of 30%, and an extended fluorescence lifetime of 6.4 ns. The hybrid retains its optical characteristics for more than 30 days, demonstrating excellent aqueous and photostability.

The PFN enables ultrasensitive detection of 4-nitroaniline and 2,4-dinitroaniline with detection limits of 1.4 and 1.5 ppb, respectively, through $NH_2$–$Zn^{2+}$ coordination, ground-state complexation, and static fluorescence quenching [2]. Successful sensing in tap and river water highlights its practical potential. Remarkably, the nanocomposite exhibits synergistic antibacterial activity against Staphylococcus aureus and Pseudomonas aeruginosa, with $MIC_{50}$ values of 0.029 ± 0.002 and 0.020 ± 0.001 µg $mL^{-1}$, respectively. Furthermore, approximately 85–90% cell viability and strong intracellular fluorescence demonstrate its potential for high-resolution bioimaging and future theranostic applications [1]. Overall, this multifunctional PFN bridges ultrasensitive molecular sensing, antimicrobial defense, and bioimaging in a single stable nanoscale platform.

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**Keywords:** plasmon-enhanced fluorescence; silver nanoparticles; nitroaniline sensing; antimicrobial activity; bioimaging.

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# A Light-weight Monte Carlo Simulation Based In Silico Protein Design Method for Mutation Induced Fold Switch

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Structural plasticity of naturally occurring proteins allows them to change their shape in response to environmental factors such as pH, temperature, or binding partners. This ability to adopt different conformations is essential for many biological processes. While computational methods have been applied to design and redesign protein sequences that fold to a single ordered and stable state, the computational design of protein sequences with high sequence similarity that adopt well-defined but structurally divergent structures remains an outstanding challenge. Here, we designed 28 pairs of sequences using Monte Carlo simulation, denoted as (a1, b1), (a2, b2), (a3, b3), ..., (a28, b28), where ai and bi represent sequences adopting the 3-α fold and 4β + α fold, respectively. Among these, we identified three sets of foldswitching protein sequences, (a1, b1), (a2, b2), and (a3, b3): one with 89.29% sequence similarity and two others with 87.50% sequence similarity. This reflects the ability of statistical potential to finely balance competing structural constraints. The designed sequences differ by only a few residues; however, they possess different tertiary structures: a 3-α helix fold and a 4β + α fold. In addition, sequence variants for a1, a2, and a3 are also rationally designed, and the results show striking outcomes: single point mutations, specifically D26C or A39F in a1, are sufficient to induce fold switching from the 3-α fold to the 4β + α fold while maintaining 98% sequence similarity with the parent sequence.

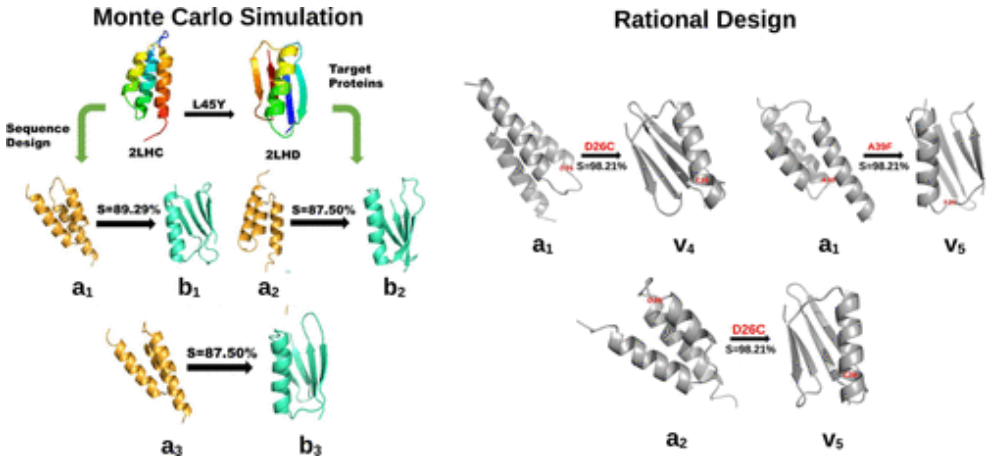



**Figure 1.** Computational design of single or pair mutation induced fold switch proteins

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**Keywords:** Protein design; fold switch; Monte Carlo simulation

# Ligand-driven entropic collapse directs mechanical strain to facilitate BirA dimerization

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The bifunctional *Escherichia coli* biotin repressor (BirA) operates as a classic allosteric switch [1,2], where corepressor binding at a highly flexible active site induces homodimerization at a spatially distant interface [3]. Because static crystallography inherently obscures the thermodynamic penalties associated with disorder-to-order transitions [4,5], the mechanical conduit connecting the localized active site [6] (L1 and L5 loops) to the distant dimerization interface (L2 and L4 loops) has remained unresolved [7]. Here, we utilize microsecond-scale all-atom molecular dynamics simulations coupled with information theory, perturbation-response scanning, and dynamical network analysis to explicitly map the allosteric pre-organization of the BirA monomer. We demonstrate that substantial enthalpic stabilization by the corepressor drives a highly targeted entropic rigidification of the active-site loops. Crucially, this localized loss of flexibility is mitigated by a compensatory entropic release at the L2 interface. Acting as a thermodynamic shock absorber, this flexibility allows the L2 loop to undergo a dynamic contact exchange, sliding along a newly exposed hydrophobic track on the core rather than freezing into a rigid, dimerization-incompetent conformation. Network and linear-response analyses reveal that this spatial repositioning is driven by a convergent mechanical routing: the L5 canopy leverages against a rigidified L1 structural strut, funneling strain directly through a discrete β-barrel bottleneck (Leu188) before terminating precisely at the L2 docking track (Leu139). By consolidating these discrete communication routes, ligand binding pays the dominant configurational cost of active-site rigidification within the monomer while producing a local contact rearrangement at the L2 loop, thereby facilitating subsequent dimerization while preserving interfacial flexibility and exposing novel cryptic core vulnerabilities for targeted mutagenesis and allosteric drug design.

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**Keywords:** allostery; molecular dynamics simulation; configurational entropy; biotin repressor (BirA); dynamical network analysis

# Unravelling PNIPAM Hysteresis: A Solvent Relaxation NMR Study of the Globule-to-Coil Transition

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The well-known homopolymer Poly(N-isopropylacrylamide) (PNIPAM) exhibits a thermally induced coil-to-globule transition in aqueous media near its lower critical solution temperature (LCST). Previous studies have established the hysteresis between the coil-to-globule and globule-to-coil transitions and have explained this behaviour through structural rearrangements, changes in hydration environments, and intrachain interactions in the globular state [1]. However, a quantitative and detailed investigation of the reverse transition through the dynamics of the surrounding solvent and solute–solvent interactions remains relatively unexplored.

In our previous work, we demonstrated that solvent-relaxation NMR can effectively monitor the PNIPAM coil-to-globule transition, characterized by a distinct jump in the relaxation time of water, which was quantitatively described using a theoretical model [2]. In the present work, we extend this approach to investigate the hysteretic globule-to-coil transition during cooling. Interestingly, instead of the single distinct jump observed during the coil-to-globule transition, the water relaxation-time trajectory exhibits multiple well-defined jumps during the reverse transition. This observation suggests that the globule-to-coil transformation may proceed through multiple stages involving successive changes in solute–solvent interactions accompanied by structural rearrangements. We further modified our earlier theoretical model to describe these multiple relaxation features and extract quantitative parameters that characterize the reverse transition.

This study provides a new solvent-dynamical perspective on PNIPAM hysteresis and opens a route to quantitatively probing the molecular pathway of the globule-to-coil transition in other thermoresponsive polymers.

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**Keywords:** PNIPAM; Hysteresis; NMR Solvent Relaxation

# Gas and Aqueous Phase Oxidation of a Series of Lactones: Initiated with OH Radicals

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Lactones are an important group of oxygenated volatile organic compounds (OVOCs) that readily partition into the aqueous phase and undergo oxidation by dissolved OH radicals due to their high polarity and solubility [1,2]. Despite this, the oxidation of their aqueous phase remains unknown. Thus, we have explored the gas- and aqueous-phase oxidation of β-butyrolactone (BBL), γ-butyrolactone (GBL), and δ-valerolactone (DVL) by OH radicals, thereby enabling their direct comparison under two atmospheric conditions. The vibrational frequencies and geometries were calculated at the M06-2X/6-311++G(d,p) level; the reaction energetics were further refined using CCSD(T)/cc-pVTZ single-point calculations. The aqueous phase was mimicked by incorporating explicit water molecules together with the IEFPCM model. Temperature-dependent rate coefficients were determined employing canonical variational transition state theory (CVT) coupled with small-curvature tunnelling (SCT) corrections across a temperature range of 200 to 360 Kelvin. The oxidation of lactones occurs via a hydrogen-abstraction reaction in both phases. In the aqueous phase, the activation energy of the reaction decreased for most pathways. The calculated gas-phase rate coefficient exhibited positive temperature dependence, whereas the trend reversed in the aqueous phase, primarily due to enhanced stabilization of pre-reaction complexes. The gas-phase rate coefficient follows the order BBL < GBL < DVL, while the aqueous-phase reactivity changed to BBL < DVL < GBL, demonstrating that solvation can substantially alter the relative reaction kinetics of lactones. The atmospheric lifetimes are shorter in the aqueous phase, indicating that uptake of lactones in the aqueous phase can play a major role in their atmospheric degradation.

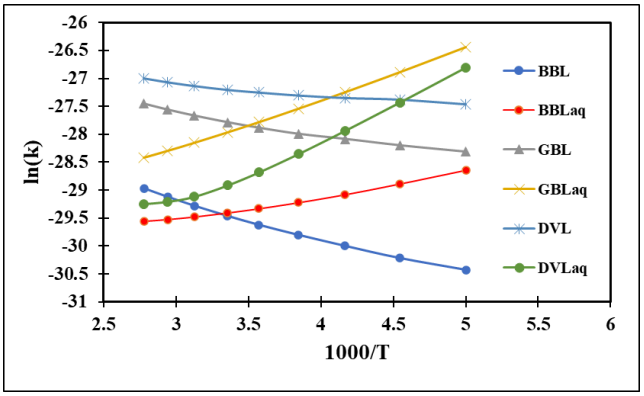



**Figure 1.** Computed total rate coefficients for BBL, BBLaq, GBL, GBLaq, DVL, and DVLaq oxidation in the 200–360 K temperature range at the M06-2X/6-311++G(d,p) level of theory.

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**Keywords:** oxygenated volatile organic compounds; lactones; multiphase oxidation; aqueous phase; reaction kinetics; atmospheric lifetimes

# A Sustainable and Catalyst-Free Direct Photochemical Route for the Conversion of Amines to Imines via C–N Coupling Reaction Under Ambient Conditions

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The elementary photophysical processes governing catalyst-free photochemical oxidation of amines remain inadequately understood. Herein, we uncover an inherent yet previously overlooked photoexcitation pathway that enables the direct conversion of amines to imines under near-UVA irradiation ($\lambda_{ex}$ = 370 nm) and ambient conditions. Ultraviolet–visible spectroscopy reveals negligible absorption of amines in the near-UVA region, whereas neat oxygenated solvents exhibit a weak, broad absorption tail. We attribute this feature to charge-transfer (CT) excitation of transient solvent–triplet oxygen (solvent–$^3O_2$) collision complexes. Charge-transfer (CT) excitation generates singlet oxygen ($^1O_2$, $a^1\Delta g$) in situ without external photosensitizers, photocatalysts, or stoichiometric oxidants, as established by characteristic $^1O_2$ phosphorescence and electron paramagnetic resonance (EPR) spin-trapping measurements. The photogenerated $^1O_2$ subsequently oxidizes amines through a single-electron-transfer pathway, generating amine radical cations and superoxide radical anions that evolve through iminium intermediates toward oxidative C–N coupling and imine formation. The reaction proceeds selectively under ambient air, with hydrogen peroxide and ammonia generated as byproducts. Systematic investigation of solvent environment, oxygen availability, and excitation wavelength establishes a direct relationship between solvent–oxygen CT excitation and photochemical reactivity. These findings reveal solvent–oxygen charge-transfer excitation as a fundamental sensitizer-free pathway for reactive oxygen species generation and provide a photophysical framework linking molecular excitation, excited-state processes, electron-transfer dynamics, and chemical transformation.

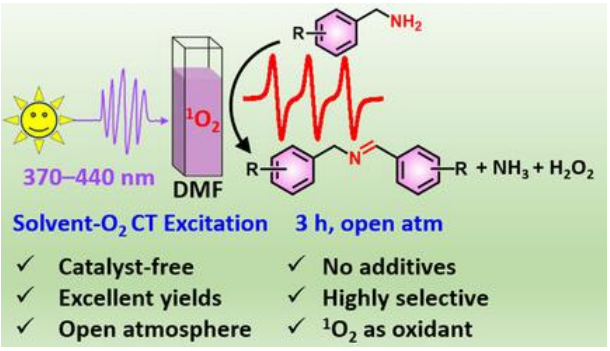



**Figure 1.** Photochemical conversions of Amines to imines

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**Keywords:** Catalyst-free photochemistry; Solvent–oxygen charge transfer; Singlet oxygen; Reactive oxygen species; Photophysical mechanisms; Excited-state dynamics

# Effect of Protein on Photoisomerization of Bacteriophytochrome

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Phytochromes are light-sensing proteins found in bacteria and plants that regulate a wide range of biological processes in response to light [1]. Their function involves reversible photoisomerization of a bilin chromophore between two forms, the cis-Pr and trans-Pfr states. Despite extensive experimental and theoretical efforts, the molecular mechanism of this photoconversion and the role of the protein environment in controlling the reaction remain incompletely understood. A detailed understanding of this process is important for exploiting phytochromes in applications ranging from crop improvement to fluorescent imaging [2].

Here, we investigate the mechanism of phytochrome photoisomerization using state-of-the-art quantum mechanical (QM) methods and hybrid quantum mechanics/molecular mechanics (QM/MM) approaches [3]. We map the energetics of the photoisomerization pathways within the protein environment and identify key stationary points on the excited-state potential-energy surface. Our results demonstrate that the protein environment plays a crucial role in determining the direction of chromophore rotation, thereby influencing the outcome of both the forward and reverse photoconversion pathways. These findings provide a molecular-level picture of how the protein controls photochemical reactivity and highlight the importance of explicitly accounting for the surrounding protein environment when describing phytochrome photocycle dynamics. The work provides mechanistic insight into the origin of directional photoisomerization and may aid the rational design and engineering of phytochrome-based applications.

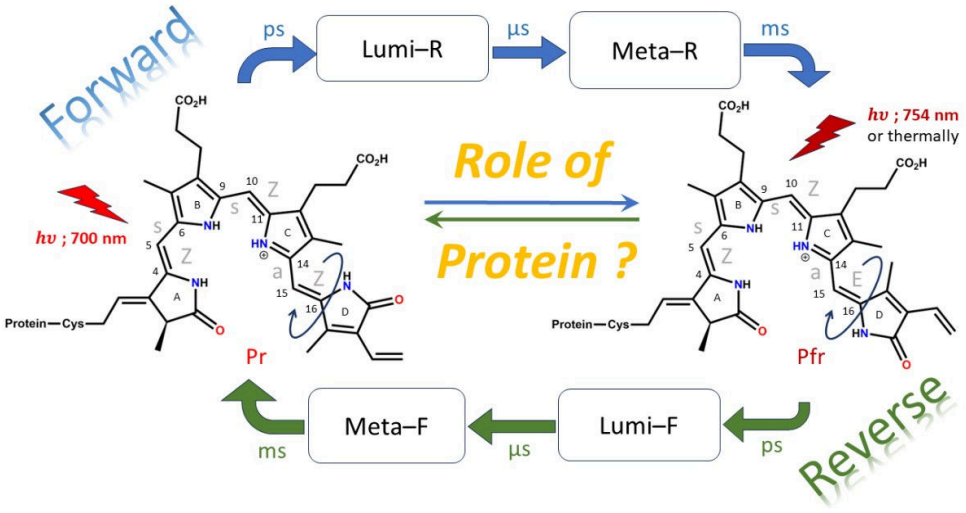



**Figure 1.** Schematic representation of photocycle of bacteriophytochrome photoreceptor.

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**Keywords:** Phytochrome; Photoisomerization; QM/MM; Excited-state.

# Tailoring Quantum Dot Properties for Quantum Science: Influence of Charge, Energy Transfer and Anisotropy on Exciton Dynamics in Quantum dots and their Assemblies

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Excitons, formed when light creates a bound electron–hole pair in a semiconductor nanocrystal, determine how quantum dots (QDs) absorb and emit light. At QD interfaces, the exciton dynamics influence the performance of nanocrystal-based optoelectronic devices. In layered assemblies, these dynamics are governed not only by intrinsic material properties, but also by interfacial processes such as charge transfer (CT) and Förster resonance energy transfer (FRET). Heterostructures composed of emissive I-III-$VI_2$ nanocrystals (e.g., $CuInS_2$/ CdS) and non-emissive $CuFeS_2$ layers exhibit competitive interfacial interactions shaped by Fermi level offsets and electronic coupling. [1] These I-III-$VI_2$ quantum dots exhibit large Stokes shifts, suppressing reabsorption and enhancing optical transparency- an important feature for applications such as transparent displays and lighting. We demonstrated that proximity-induced Fermi level shifts and interlayer band bending play a decisive role in determining whether FRET or ground-state CT dominates. These competing pathways can significantly alter emission intensity and lifetime, revealing how interfacial energetics can be used to control optical quenching and charge separation in QD assemblies. Our findings highlight that exciton dynamics in I-III-$VI_2$ heterostructures can be engineered through the design of interfacial band structure and carrier localization.1 The results provide a conceptual framework for using band-edge structure and local strain to tune excitonic interactions in QD architectures.

We further discuss the incorporation of anisotropic core/shell quantum dots into these assemblies. These materials offer a route to tailor excitonic fine structure and exciton-phonon interactions in quantum dot heterostructures. [2,3] We develop and compare two types of ZnTe-based heterostructures: conventional ZnTe/ CdS with symmetric shells and asymmetric structured ZnTe/ CdS. We study how geometric asymmetry influences radiative lifetimes, exciton dynamics, and emission linewidths at both ensemble and single-particle levels. This work builds on the conceptual foundation established in I-III-$VI_2$ systems and extends it to fine structure engineered quantum dots for advanced optoelectronic applications.

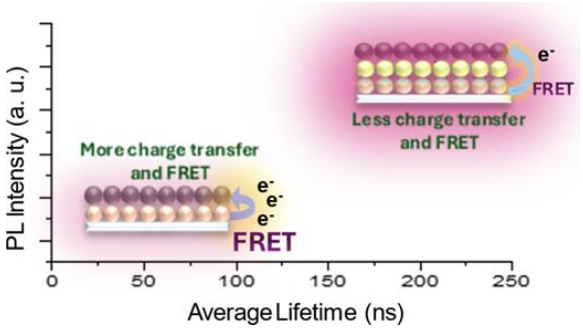



**Figure 1.** Charge transfer and FRET are governed by interfacial proximity and influence exciton lifetime and PL intensity.

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**Keywords:** quantum dots; exciton dynamics; excitonic fine structure; exciton-phonon interaction

# Unveiling the Influence of Biomolecules on the Relaxivity of Mn(II) Based Contrast Agents: A Molecular Dynamics Study

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Magnetic Resonance Imaging (MRI) is a non-invasive imaging technique that primarily uses a strong magnetic field to split water protons into lower and higher energy states, and a radio frequency pulse to excite them. However, to obtain a high-contrast image, this technique typically uses a metal-centred complex called contrast agent (CA) that acts as a localized magnet, thereby enhancing proton relaxation in water molecules.[1] However, a recent study reveals that the commonly used Gadolinium based contrast agents (GBCAs) have numerous side effects.[2] Therefore, there is a demand for an alternative non-toxic contrast agent. As an alternative, Mn(II) based CAs have emerged as a potential replacement in recent years. The relaxivity (efficiency) of a CA is mostly contributed by the inner sphere water molecule,[3] which undergoes frequent exchange with the bulk water. Therefore, our study mainly focuses on the inner sphere water molecule and its intrinsic parameters, such as the metal ion to oxygen distance (IOD) and residence time. In this context, we have utilized parameterized atomistic classical simulations on Mn(II) CAs. Furthermore, we have used these parameterized topologies to study the influence of biomolecules on relaxivity. Overall, we have found that the presence of biomolecules such as HSA protein drastically alters the rotational correlation time of the CAs, changing it from the picosecond scale to the nanosecond scale.[4] It also influences water dynamics by occupying spatial positions and altering water residence time.[4] The computational approach and the outcomes of this study can be utilized to develop novel Mn(II)-based CAs specifically designed to target biomolecules, thereby further enhancing relaxivity.

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**Keywords:** MRI, Contrast Agent, Relaxivity, Classical Simulation

# Raman Spectroscopic Investigation of Biochemical Changes in Imiquimod-Induced Psoriasis Model

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Psoriasis is a chronic inflammatory skin disease that is characterised by keratinocyte hyperproliferation, skin erythema and changes in the lipid and protein composition of the epidermis layer. Conventional diagnostic techniques for disease monitoring are mainly based on histopathology, which is invasive and does not reflect real-time biochemical changes. Raman spectroscopy is a vibrational spectroscopic technique based on inelastic scattering as light interacts with the vibrational modes of chemical bonds in molecules, providing a label-free, non-destructive means of probing molecular-level changes and is therefore a promising tool for characterising disease progression in psoriasis models. In our study, Raman spectroscopy was used to investigate biochemical changes accompanying the IMQ-induced psoriasis-like mouse model. Inflammation was chemically induced in BALB/c mouse ears using Imiquimod cream, and ear skin tissue and blood serum were collected post-inflammation. Raman spectra of ear tissue and serum were collected using a 785nm excitation laser to determine biochemical changes at the site of inflammation and understand the systemic inflammatory response, respectively. A machine learning method known as Partial Least Squares Discriminant Analysis (PLS-DA) was applied to classify spectra and identify spectral markers associated with inflammation.

In lesional ear tissue, the bands specific to collagen (870, 937, 1652 $cm^{-1}$) were less intense than in controls, indicating collagen degradation that occurred during the development of psoriasis-like inflammation. Moreover, haemoglobin-associated peak (667 $cm^{-1}$) appeared in lesional ear tissue spectra, which corresponds to the development of skin erythema. Serum spectra revealed distinct alterations in protein-associated bands, indicating changes in serum protein composition consistent with a systemic inflammatory response. These findings suggest that Raman spectroscopy can be used to detect both local and systemic biochemical signatures of psoriatic inflammation, supporting its potential as a label-free, non-destructive, rapid tool for monitoring disease progression and therapeutic response in psoriasis models.

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**Keywords:** Raman Spectroscopy; Psoriasis; Skin Inflammation; Machine learning; skin biochemistry.

# From Core Insertion to Surface Binding: A Molecular Dynamics Study of $hCT_{10-22}$ Fragment Behavior on Different Lipid Membranes

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Human Calcitonin (hCT) is a therapeutic peptide used in calcium and phosphate metabolism. However, due to its propensity towards fibril formation (associated with thyroid carcinoma), its clinical application has been discontinued. There are several studies on inhibiting the aggregation of hCT, yet its interactions with different membranes remain insufficiently understood. In our work, we have studied the interaction of the $hCT_{10-22}$ fragment monomer with two different membrane types: a pure zwitterionic DOPC membrane and a 7:3 DOPC-anionic membrane mixture. Using molecular dynamics simulations, we have compared the conformational behavior and insertion depth of this peptide fragment as well as membrane dynamics in these two systems. A significant difference has been observed between two membrane environments. In the pure zwitterionic DOPC membrane, the peptide inserts readily into the membrane's hydrophobic core while maintaining a higher order helicity. In contrast, in the mixed bilayer system, the peptide remains localized on the bilayer surface and is unable to penetrate the densely packed lipid structure with reduced helicity, indicating that surface interactions with the anionic lipid headgroups change its helical structure. However, in both bilayer systems, the relative orientation of the peptide with respect to the bilayer membrane remains largely unchanged, ruling out major structural reorientation. These findings explain that the difference in lipid composition changes the peptide accessibility- a key factor governing the aggregation pathways and provides molecular-level insights for therapeutic development.

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# Investigation of the interactions of influenza A virus-encoded miRNA with human PCBP2 mRNA and Agronaute-2 protein at the single-molecule level

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MicroRNAs (miRNAs) play a crucial role in regulating cellular gene expression by interacting with target mRNAs through association with argonaute (Ago) proteins. Recently, a miRNA from the highly pathogenic avian influenza virus type A H5N1, known as miR-HA-3p, was shown to target host mRNA encoding poly(rC) binding protein 2 (PCBP2) [1]. PCBP2 plays a crucial role in the defense mechanisms against viruses and in preventing excessive cytokine production. However, a comprehensive biophysical characterization of miR-HA-3p folding-unfolding properties, and its interaction with PCBP2 mRNA and the role of Ago-2 in this is still lacking.

Here, we report a fluorescence-based investigation of the folding and unfolding properties of a Förster resonance energy transfer (FRET)-paired miR-HA-3p, as well as its interactions with the PCBP2 mRNA segment it specifically targets and with human Ago2 (hAgo2). Furthermore, we present single-molecule investigation on FRET-miR-HA-3p using two-dimensional fluorescence lifetime correlation spectroscopy (2D FLCS) [2, 3] to resolve the distinct conformational states of the miRNA and their interconversion dynamics with a temporal resolution of 2 microseconds in different conditions, viz. in the single-stranded form and when bound to target mRNA/protein.

Our observations indicate that the single-stranded miR-HA-3p exists in multiple compact, folded structures that interconvert on the microsecond to millisecond time scale. Upon binding to the PCBP2 mRNA and hAgo2 protein with nanomolar affinities, miR-HA-3p primarily adopts extended structures, with limited structural interconversions occurring on the microsecond timescale within the miRNA-mRNA and miRNA-protein complexes. These findings provide valuable insights into the conformational states and dynamics of miR-HA-3p and its interactions with its host mRNA target and protein, contributing to a better understanding of the molecular mechanisms of gene regulation by this virus-encoded miRNA.

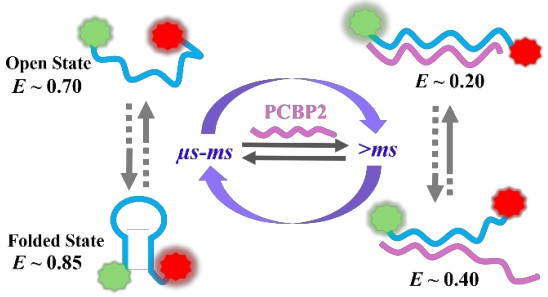



**Figure 1.** Schematic representation of the binding of FRET-miR-HA-3p to PCBP2 mRNA and its conformational dynamics in the single-stranded form (left) and in the target-mRNA-bound form (right).

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**Keywords:** Conformational dynamics, virus-encoded microRNA, 2D FLCS

# Committor-Based Detection of Post-Transition-State Bifurcations from Enhanced-Sampling Simulations

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Post-transition-state bifurcation (PTSB) reactions, where a single transition state connects to multiple products through dynamically controlled branching beyond the barrier, defies the conventional transition-state theory, which assumes that one transition state yields one product. Such reactions rely on minimum-energy paths blind to the orthogonal, momentum-dependent coordinates that govern branching. Because the competing product channels can share nearly identical values of the biasing collective variables (CVs), enhanced-sampling schemes built on a single minimum-energy pathway cannot, on their own, reveal the branching: the CV-based reaction coordinate gives an incomplete picture.

We demonstrate a recently proposed committor-based framework for detecting bifurcation pathways directly from enhanced-sampling trajectories. Variational committor networks (VCNs) are trained on well-tempered metadynamics eABF QM/MM sampling to learn the committor as a function of full molecular geometry rather than of the path CV alone. By allowing the individual bond distances to vary along the path and reading these orthogonal coordinates, the committor distinguishes configurations that the CV cannot. Distinct product channels are then resolved by clustering configurations within isocommittor slices requiring no prior specification of the product manifold, and the analysis yields committor-consistent reaction coordinates that improve on geometric path definitions. We apply this protocol to a cyclopentyl azide rearrangement reaction. These results establish committor networks as a practical, alternative route to mechanistic discovery in bifurcating reactions, where static transition-state theory and single-coordinate enhanced sampling are insufficient.

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**Keywords:** neural network; committor; Post Transition State Bifurcation reactions; Metadynamics

# Quantitative Pathway-Resolved Kinetics from Neural Network-Guided Weighted Ensemble Simulations

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Many crucial biomolecular processes, such as ligand dissociation and conformational switching, occur via multiple competing transition pathways. While standard rare-event sampling methods provide rigorous estimates of the global transition rate, they often collapse mechanistic heterogeneity into a single constant, obscuring the relative kinetic contributions of distinct channels. Here, we introduce a path-resolved weighted ensemble (WE) framework that quantitatively assigns steady-state flux to competing transition channels without modifying the underlying unbiased dynamics. Initial reactive trajectories are generated by direction-guided adaptive sampling, clustered by dynamic time warping (DTW), and smoothed into neural-network-refined representative paths. These refined routes are used as path collective variables (PathCVs) to pre-seed and guide channel-specific WE simulations. We demonstrate the robustness of this framework across systems of increasing complexity. On a model three-hole potential, it captures a temperature-dependent pathway crossover. In the benzamidine-trypsin complex, it isolates the dominant unbinding route while quantifying subdominant channel fluxes. Finally, for imatinib dissociation from Abl kinase, the method reveals that the clinically relevant N368S resistance mutation redistributes reactive flux from the P-loop/hinge channel toward the $\alpha$C-helix channel, accelerating escape. This framework transforms qualitative pathway classification into rigorous, pathway-specific kinetic observables, providing a powerful route to understanding mutation-induced mechanistic shifts in biomolecular function.

**References**

**Keywords:** weighted ensemble; path collective variables; rare-event sampling; biomolecular kinetics; pathway-resolved flux

# Mechanistic Role of Different Functional Groups in Inhibiting Tryptophan Self-Assembly: Comparison between Aromatic and Nonaromatic Hydroxyl Moiety-Rich Chemical Compounds

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Tryptophan (TRP) self-assembly is responsible for the development of several neurodegenerative disorders, such as hypertryptophanemia, for which effective therapeutics are still lacking. Although several experimental studies have demonstrated varying inhibitory efficacies of different functional moiety-rich compounds, the mechanistic role of individual functional groups while inhibiting the spontaneous self-assembly is still elusive. We have performed molecular dynamics simulations to explore different kinds of interspecies interactions between TRP and distinct functional groups present in experimentally studied aromatic and nonaromatic compounds with varying concentrations: tannic acid (TA), which contains both aromatic and hydroxyl moieties, and polyols, namely, sorbitol and mannitol, which contain no aromatic ring but only hydroxyl moieties. TA reduces TRP self-assembly more effectively than polyols, a difference not attributable solely to molecular size or multivalency. Quantitative analyses of different TRP–TA interactions, including π–π stacking between aromatic rings and H-bonding between respective hydroxyl moieties, reveal that lifetimes of π–π stacking are much higher than the H-bond lifetimes. Notably, the number and strength of π–π stacking interactions dominate over the H-bonding interaction in TA-mediated inhibition, although a large number of hydroxyl groups are present in TA. Consequently, TRP exhibits longer residence times in the vicinity of TA than polyols. Furthermore, TA weakens π–π stacking between TRP molecules, reducing TRP aggregation. The computed TRP–TA binding energy may therefore serve as a guide for evaluating the efficacies of other chemical compounds, demonstrating the importance of the aromatic ring in inhibiting the early stages of TRP oligomerization.

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**Keywords:** Tryptophan self-assembly; molecular dynamics simulations; π − π stacking; intermolecular interactions; aggregation inhibition

# Stochastic Thermodynamics of a Non-Markovian Random Process

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Understanding thermodynamics of non-equilibrium systems at the microscopic level is a rapidly growing field of research[1,2]. This field has led to the emergence of a new field of research of stochastic thermodynamics, which aims to study thermodynamic aspects of microscopic system influenced by thermal fluctuations. We discuss thermodynamic aspects of a recently studied non-Markovian process[3] where memory effects manifest in terms of time-dependent harmonic potential and gives rise to trajectory-dependent stochastic work and heat. The memory-driven potential can be bound or unbound depending upon how the process depends on its memory. Based on memory-driven potential, we define work done, heat dissipation, and entropy production; and those depend on memory strength parameter. We derive exact form of the moment generating function of work done and entropy production to better understand stochastic behavior of these thermodynamic quantities. We analyze the work fluctuation theorem and thermodynamic uncertainty relations and show that the latter holds true only for the unbound potential, for bound potential it is violated at long times which depends inversely on the width of the initial position distribution.

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**Keywords**: Stochastic Thermodynamics; Non-Markovian; Memory; Non-Equilibrium; Fluctuations

# Therapeutic Targeting of Cancer-Associated PKM2 Mutants by Shikonin via Mutation-Induced Pocket Recognition

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Pyruvate kinase (PKM2) is a key glycolytic enzyme involved in cancer metabolic reprogramming and frequently harbors oncogenic missense mutations that alter its structural and functional dynamics [1]. Here, we investigate the molecular basis of recognition of the anti-cancer drug shikonin in wild type (WT) and six PKM2 mutants. Molecular docking identified three mutants (R246S, P117L, H464A) exhibiting favourable binding of shikonin within a newly identified pocket adjacent to the allosteric site, while the WT accomodated shikonin in the known active site pocket, consistent with previous literature reports. Subsequently, 1 µs MD simulations confirmed reduced conformational fluctuations, higher $\Delta G^{o}_{bind}$ values and persistent residue contacts in these mutants, whereas the other three mutants (K367M, R399E, R455Q) displayed disrupted pocket integrity, lower $\Delta G^{o}_{bind}$ values and unstable ligand binding. $R_g$ , PCA, Fpocket program and residue communication network analyses revealed that the favourable binding mutants maintain a compact pocket architecture stablized through efficient short-range allosteric coupling between the mutation sites and pocket residues and druggability scores greater than 0.5, while weak-binding mutants showcase weakened long-range communication pathways. Interaction profiling further identified stable hydrogen bonding and stacking interactions supported by favourable interaction energies. Overall, this study demonstrates that PKM2 mutations dynamically remodel the binding pocket and allosteric communication to facilitate shikonin recognition and highlighting the newly identified pocket as a promising therapeutic site for future PKM2 targeted drug design.

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**Keywords:** Pyruvate Kinase, PKM2, Shikonin, PKM2 Mutants, Anti-cancer

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# Computational Investigation of Through-Bond and Through-Space Charge Transfer for Reduced or Inverted $\Delta E_{ST}$ in TADF Emitters

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Thermally activated delayed fluorescence (TADF) offers a promising strategy for realizing highly efficient organic light-emitting diodes by enabling triplet excitons to contribute to light emission through reverse intersystem crossing (RISC). A key molecular descriptor governing this process is the singlet–triplet energy gap ($\Delta E_{ST}$), which is strongly influenced by the exchange interaction and, consequently, by the spatial distribution and electronic coupling of donor and acceptor states. Here, we investigate donor–spacer–acceptor architectures as a systematic platform for controlling charge-transfer topology and tuning $\Delta E_{ST}$ toward exceptionally small and inverted values. The molecular structures are designed to independently modulate donor–acceptor conjugation, spatial proximity, and torsional geometry, thereby enabling comparison of through-bond charge transfer (TBCT) and through-space charge transfer (TSCT). Extended π-conjugation is employed to enhance through-bond electronic coupling, whereas spatially proximate but electronically decoupled donor–acceptor units are used to promote through-space interactions. This framework enables the relationship between molecular geometry, orbital coupling, charge-transfer character, and singlet–triplet energetics to be examined systematically.

Ground- and excited-state electronic structures are investigated using density functional theory (DFT) and time-dependent DFT (TDDFT), with particular emphasis on the energetic and electronic characteristics of the lowest singlet and triplet excited states. The dependence of $\Delta E_{ST}$ on donor–acceptor separation, torsional configuration, conjugation, and charge-transfer character is evaluated alongside oscillator strengths and spin–orbit coupling. The resulting excited states are analyzed to distinguish TBCT- and TSCT-dominated configurations and to identify structural factors that govern their photophysical properties. By establishing structure–property relationships between charge-transfer topology, electronic coupling, and $\Delta E_{ST}$, this work seeks to clarify the molecular mechanisms governing singlet–triplet-gap reduction in donor–acceptor TADF systems. The study provides a computational framework for identifying structural motifs capable of simultaneously controlling charge-transfer character and excited-state energetics, thereby guiding the rational design of next-generation TADF emitters with small or inverted $\Delta E_{ST}$.

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**Keywords:** TBCT; TSCT; TADF; Singlet Triplet Energy Gap; DFT

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# Estimation of Absolute Protein–DNA Binding Free Energy using Streamlined Geometric Formalism

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Protein-DNA complexes are involved in vital cellular functions like gene regulation, replication, transcription, packaging, rearrangement, and damage repair. In this work, we proposed an intricate streamlined geometric formalism for computing the absolute binding free energy, which can be used to obtain chemically accurate in silico estimation of the binding free energy of three Protein-DNA complexes. In the formalism, a series of potential of mean force, using hybrid Gaussian-Accelerated Well-Tempered Metadynamics-Extended Adaptive Biasing Force sampling method (GaWTM-eABF), were performed while harmonically restricting the positional and orientational degrees of freedom involving bound states of the complex, hence attenuating the configuration entropy available to the system and alleviating the sampling limitations. Enhanced Sampling technique for free energy estimation, popularly known as BFEE2 (Binding Free Energy Estimator 2) [1] could be employed for DNA bounded protein complexes. Additionally, analysis of molecular interactions between protein and DNA molecules paints a picture in which hydrogen bonds, electrostatic, van der Waals, pi-cation, and hydrophobic interactions were primarily responsible for the association of the protein-DNA complex. Using this formalism, one can obtain the absolute binding free energy for a Protein-DNA complex with remarkable accuracy and modest computational cost. [2]

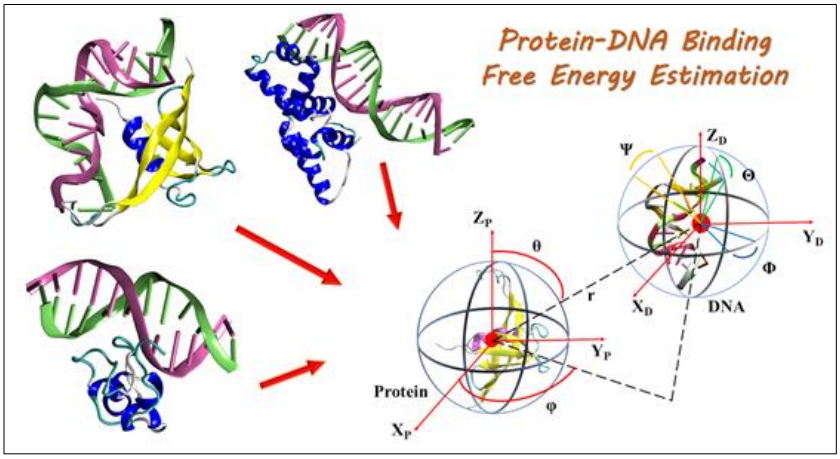



**Figure 1:** Representation of complexes (a) CFP1-CpG Complex, (b) MC1-DNA Complex, and (c) SopB-DNA Complex; where, both protein and DNA are represented using New Cartoon representation and colored according to the secondary structure and chains, respectively.

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**Keywords:** BFEE2 (Binding Free Energy Estimator 2); MC1-DNA complex; SopB-DNA complex; CFP1-CpG Complex.

# Mg-Co-B Chemical Space for Mg-Ion Cathodes: Evolutionary Search, Machine Learning, and Chemical Bonding Analysis

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## Abstract

The growing demand for high-performance energy storage systems has increased interest in alternatives to conventional Li-ion batteries. Among the proposed post Li-ion technologies, Mg-ion batteries are particularly attractive because magnesium is abundant and offers a higher volumetric capacity than lithium. Their practical development, however, is hindered by the sluggish migration of $Mg^{2+}$ ions, which arises from their strong interaction with the surrounding host lattice and can lead to poor ionic conductivity and limited reversible capacity. Here, we investigate the Mg-Co-B chemical space using an evolutionary structure-search approach combined with convex-hull analysis. Three thermodynamically stable compounds, MgCoB, $MgCo_3B_2$, and $Mg_3Co_3B_2$ were identified. Extensive computational analyses was further deployed through phonon dispersion calculation, Gibbs free-energy analysis and formation energy calculations. To explore the large number of symmetry-inequivalent structures generated during Mg extraction, a machine learning interatomic potential for efficient structural screening was employed, followed by DFT calculations to obtain reliable energetics. This combined approach considerably reduces the computational effort associated first-principles calculations. The electrochemical properties and chemical bonding characteristics of the identified compounds were subsequently examined using DFT calculations. $Mg_3Co_3B_2$ undergoes significant structural destabilization upon demagnesiation, making it unsuitable as a cathode. Although $MgCo_3B_2$ remains structurally viable, its relatively high $Mg^{2+}$ migration barrier of 0.75 eV is expected to hinder Mg-ion transport. MgCoB on the other hand, shows a more favourable combination of electrochemical and transport properties, with a theoretical specific capacity of 356.2 mAh $g^{-1}$, a gravimetric energy density of 278 Wh $kg^{-1}$ and a substantially lower $Mg^{2+}$ migration barrier of 0.35 eV. Taken together, these results depicts MgCoB as a promising candidate for Mg-ion battery cathodes and demonstrate the potential of combining evolutionary structure prediction, machine learning based structural exploration and first-principles calculations for discovering multivalent-ion battery materials.[1]

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## Keywords

Density Functional Theory, Mg-ion Battery, Mg-ion Cathode, Energy Storage Materials,

# Turning Heat into Electricity: Driving High ZT through Soft Phonon Engineering

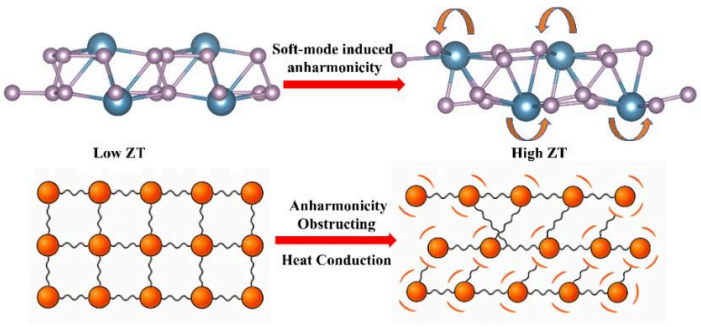
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In recent years, thermoelectric (TE) materials have attracted attention due to their ability to convert waste heat into electricity. TE materials can be used to generate electricity from temperature gradients (Seebeck effect) and cooling applications (Peltier effect). Through first-principles calculations and using the Boltzmann transport equation, we explore the TE properties of low-dimensional $MX_3$ (M = Ca, Ba and X = P, As) type compounds. Due to quantum confinement effects, these low-dimensional materials show exceptionally high figures of merit (ZT). The lattice thermal conductivities of these materials are low, whereas their electrical conductivities and Seebeck coefficients ($S$) are high, which makes them suitable candidates for applications in TE materials. We also observe that the soft phonon modes in materials can lower the lattice thermal conductivity ($\kappa_l$) and thereby increase their TE performance. Our results show the anisotropic figure of merit (ZT) for $CaP_3$ and the unexpectedly high ZT for $BaP_3$ and $CaAs_3$ at room temperature. On the other hand, $BaAs_3$, being electron-rich, shows high ZT at higher carrier concentrations and temperatures. This work provides insightful results and a mechanism for obtaining highly efficient TE materials.

**Keywords:** Two-dimensional materials; Soft-phonon modes; thermoelectric materials; Power factor; Thermal conductivity.



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# Molecular Insights and Predictive Models for Solvent Selection in Lignin Valorization

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Lignocellulosic biomass is an abundant and renewable alternative to petroleum feedstocks for fuel and chemicals. It primarily consists of cellulose, hemicellulose, and lignin; cellulose and hemicellulose have been extensively studied for biofuels and paper industries, while lignin is the most abundant natural source of aromatic monomers for the polymer and chemical production [1,2]. However, lignin valorization is challenging because of its complex heteropolymer structure and broad molecular weight distributions. Reductive catalytic fractionation (RCF) is a promising lignin-first approach that can produce high yields of phenolic monomers and oligomers [3]. RCF in an alcohol solvent over a heterogeneous Pd/C catalyst has been found to favor the generation of product mixtures that can be microbially converted to valuable products at high yield [4]. An important choice in optimizing RCF is the selection of solvent; however, there is a lack of detailed information regarding how solvent selection impacts lignin behaviors and interactions.

In this work, we performed all-atom MD simulations of an oligomeric lignin model compound in organic solvents including methanol, ethanol, ethanol+water (85:15, v:v), and water at both the RCF reaction temperature (473 K) and room temperature. Organic solvents favorably solvate lignin and promote more extended conformations compared with water, potentially increasing accessibility for catalytic conversion. Unbiased simulations incorporating model Pd and C surfaces revealed strong adsorption of lignin on both Pd and C surfaces at 473 K. Our results further indicate solvent-dependent differences in interfacial behavior, with adsorption driven by the entropy gain associated with liberation of solvent molecules from the surface [5]. Building on these molecular insights, we developed a computational solvent screening framework by correlating empirical solvent descriptors such as Hansen Solubility Parameters (HSPs) with experimental monomer and downstream product yields. This work demonstrated that hydrogen-bonding interactions play a dominant role in enhancing lignin depolymerization and product yields [6].

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**Keywords:** Lignocellulosic biomass; Lignin-surface interactions; Adsorption

# Molecular Engineering of Antiaromatic Orangarin-based Sensitizers for High-Performance Dye-Sensitized Solar Cell Applications

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Over the past few decades, solar energy has distinguished itself as an effective renewable energy source due to its relative abundance, accessibility and sustainability. Dye-sensitized solar cells (DSSCs) have become popular due to their low fabrication cost, mechanical flexibility and spectral tunability. Amongst the many organic molecules which have been used as absorbers for DSSCs, porphyrin-based dyes have stood out due to their strong light absorption, easy structural modifications and high-power conversion efficiencies. While many porphyrin-based dyes have been studied extensively, structural analogues of porphyrins are yet to be explored significantly. In this work, we designed and conducted a thorough computational investigation of orangarin derivatives as dyes for DSSC applications. To the best of our knowledge, this is the first study that examines metal-free, Hückel antiaromatic, expanded porphyrin molecules for DSSC applications. We implemented density functional theory and time-dependent density functional theory to investigate the relevant photophysical and photovoltaic properties of orangarin derivatives based on the donor-$\pi$-core-acceptor architecture. We report that all 10 designed dyes strongly absorb light in the visible region, show energetically favourable adsorption on the $(TiO_2)_{38}$ cluster, and possess enhanced charge-transfer characteristics [1]. Due to the antiaromatic nature of the orangarin core, the donors attached at the 7$^{th}$ position (*meso* position) lie in the inner circuit and thus contribute electron density effectively to the inner ring current [2]. This influences the respective absorption and photovoltaic properties. In conclusion, these enhanced properties may be expected to be utilized for the fabrication of high-performance DSSCs. Furthermore, these advantageous characteristics may motivate in-depth investigations of antiaromaticity and the role of structural modifications to establish structure-property relationships. Finally, we expect similar explorations of antiaromatic organic molecules for other relevant renewable energy applications.

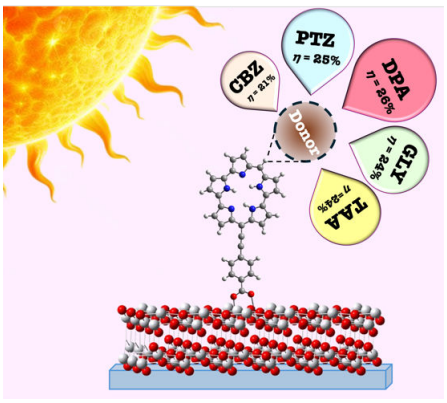



**Figure 1.** Orangarin derivatives with different electron donors for application as dyes in dye-sensitized solar cells.

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**Keywords:** Solar-energy conversion; Photovoltaics; Porphyrinoid-based dyes; Renewable energy; Optoelectronics

# Interfacial engineering of waste derived Char/$VO_2$ composites for stable electrochemical energy storage

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The development of sustainable electrode materials from waste-derived resources is important for advancing low cost and environmentally responsible electrochemical energy storage technologies. Herein, vanadium dioxide ($VO_2$) was grown in situ on waste-derived char through a hydrothermal approach, with different Char/$V_2O_5$ precursor ratios investigated to understand the influence of composition on the structural and electrochemical properties of the resulting composites. The optimized composite was identified through systematic electrochemical evaluation, where the 1:1 Char/$V_2O_5$ ratio exhibited the best overall performance, suggesting an appropriate balance between the conductive carbon framework and the redox-active $VO_2$ phase. The material was used to fabricate a two-electrode supercapacitor device. The assembled device delivered a specific capacitance of approximately 180 F $g^{-1}$ at a current density of 3 A $g^{-1}$ and demonstrated exceptional long term electrochemical stability, retaining nearly 94% of its initial capacitance after 15,000 charge/discharge cycles. The enhanced performance is attributed to the synergistic contribution of the conductive waste-derived carbon matrix and electrochemically active $VO_2$, facilitating efficient charge transport and reversible charge storage. The results demonstrate that controlling the relative composition of waste-derived carbon and $VO_2$ is critical for optimizing electrochemical performance and stability. This work therefore establishes a promising route for converting waste-derived carbon into value-added electrode materials while providing insight into composition dependent interfacial charge-storage processes in carbon/transition metal oxide systems.

**Keywords:** waste derived carbon; vanadium dioxide; supercapacitor; interfacial charge storage; electrochemical stability

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# Anti-Kasha-Type Spin-Vibronic Dynamics Drive Photoinduced Ni-H Umpolung

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Photochemical control of metal-ligand cooperation can unlock reactivity that is inaccessible on the ground-state potential-energy surface. A nickel-hydride pincer complex exhibits an unusual light-induced inversion of $CO_2$ insertion selectivity, attributed experimentally to formation of a transient Ni(0) photointermediate through Ni-H/N-H reductive elimination [1]. Here, we uncover the excited-state origin of this Ni-H umpolung using rigorous nonadiabatic excited-state dynamics together with multireference electronic-structure calculations. Photoexcitation initially prepares a bright ligand-centered singlet state, followed by ultrafast intersystem crossing into the triplet manifold on a sub-200 fs timescale. The dynamics then reveal population transfer through higher triplet states and accumulation in a long-lived $T_4$ state. Importantly, this electronic evolution is coupled to pronounced spin-vibronic nuclear motion: bending of the N-Ni-H angle and puckering of the PNP backbone progressively bring the nitrogen lone pair toward the hydride, providing the structural pathway for polarity reversal. Multireference potential-energy surfaces further show relaxation toward $T_1$ and passage through a $T_1/S_0$ minimum-energy crossing point, enabling nonradiative return to the ground state and formation of the reduced Ni(0) photointermediate. The combined dynamics and electronic-structure picture establishes an anti-Kasha-type mechanism [2] in which a higher excited-state manifold, rather than simple relaxation to the lowest excited state, controls chemical reactivity. These results highlight how coupled spin and nuclear motion can direct metal-hydride polarity inversion and provide a general mechanistic framework for exploiting excited-state metal-ligand cooperation in photochemical catalysis.

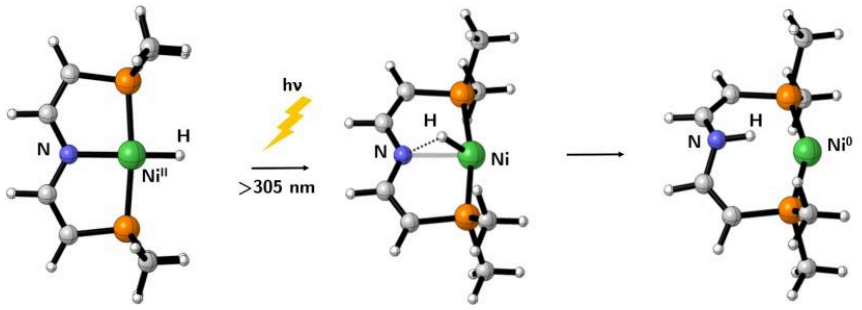



**Figure 1.** Light-induced Ni-H umpolung from a Ni(II)-hydride precursor to the Ni(0) photointermediate, highlighting the N-Ni-H bending pathway.

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**Keywords:** Anti-Kasha photochemistry; spin-vibronic dynamics; Ni-H umpolung; excited-state nonadiabatic dynamics; metal-ligand cooperation.

# Non-Markovian escape under stochastic resetting

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Stochastic resetting is a powerful strategy known to optimize target-search processes at microscopic scales[1]. While its effects on Markovian systems are well understood, its influence on memory-driven systems, such as in viscoelastic baths, has not been adequately investigated. In this work, we study the first-passage properties of escape for a harmonically trapped particle in a non-Markovian environment under stochastic resetting[2]. We employ a complete renewal approach and find that the characteristic non-exponential heavy tail of the first-passage time (FPT) distribution becomes exponential when resetting is introduced. We further find that optimal resetting is achievable at a lower reset rate when the dynamics are weakly correlated; however, for stronger correlations, the process needs to be reset more frequently[2]. Therefore, resetting in memory-driven dynamics can be used as an effective control strategy to initiate faster escape, thereby regulating efficient transport mechanisms in complex chemical and biomolecular environments that follow non-Markovian dynamics.

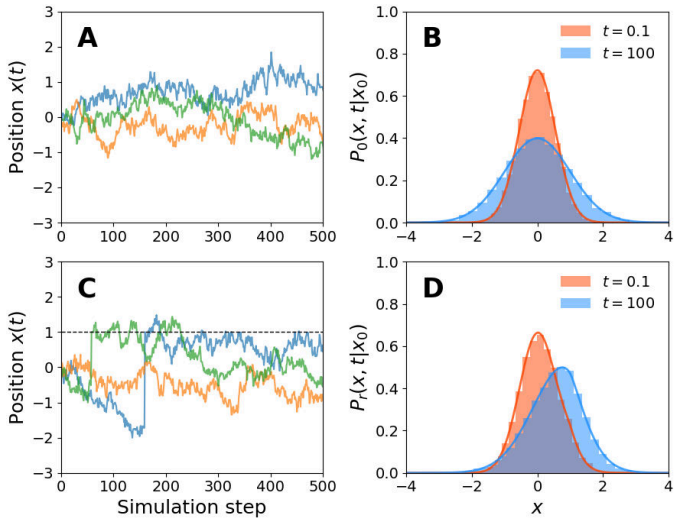



Figure 1: **Trajectories and corresponding distributions without and with resetting.** (A) Sample trajectories of particles following the dynamics described by overdamped generalized Langevin equation and fractional Gaussian noise without resetting ($r = 0$). (B) Comparison between the analytical distributions (solid lines) and simulated histograms for $r = 0$. (C) Sample trajectories showing diffusion with stochastic resetting ($r = 1$), where the jumps on the horizontal dashed line at $x_r = 1$ indicate the resetting events. The follow-up diffusive phase starts from $x_r$ after every reset. (D) Comparison between the analytical (using renewal equation) and numerical results of the probability distributions in the presence of resetting ($r = 1$). Trajectories and histograms are obtained by simulating $10^4$ trajectories with $\Delta t = 10^{-3}$, keeping $H = 0.65$ and $x_r = 1$.

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**Keywords:** Chemical kinetics; First-Passage Times; Non-Markovian Processes; Memory; Stochastic Resetting.

# Structural responsiveness as the key to water's phase behavior: Lessons from machine-learned mW and BOP models

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In most cases, water models are optimized and validated against experimental structural, thermodynamic, and dynamic properties at a single thermodynamic state, typically ambient conditions (1 bar and 298 K). However, what key ingredients should a model possess to remain transferable over a wide range of temperatures and pressures? We address this question by evaluating the original mW model and its machine-learning reoptimized counterpart, ML-mW, against experimental data and the all-atom TIP4P/2005 model over a wide range of pressures (-1000 bar to ∼4000 bar) and temperatures (218 K to 735 K), spanning all three phases of water. Our results show that ML-mW partially recovers the structural responsiveness, namely the interconversion between tetrahedral and non-tetrahedral local configurations with changes in temperature and pressure, which the original mW model severely lacks. This modest improvement in structural responsiveness leads to significant improvements in reproducing the properties of liquid water, ice–liquid thermodynamics, and vapor–liquid equilibria. In particular, ML-mW reproduces the anomalous increase in the compressibility and heat capacity of supercooled water[1] and appears to support a liquid–liquid transition (LLT) and an associated liquid–liquid critical point (LLCP)[2], features absent in the original mW model. Comparison with our previous results for the Tersoff-based ML-BOP model further shows that the transferability of a coarse-grained water model depends more on its ability to capture the structural response of water to changes in temperature and pressure than on reproducing the exact liquid structure at a single thermodynamic state. These results demonstrate that the structural responsiveness of water, together with the flexibility of the underlying functional form, is the key ingredient for developing accurate and transferable coarse-grained water models.

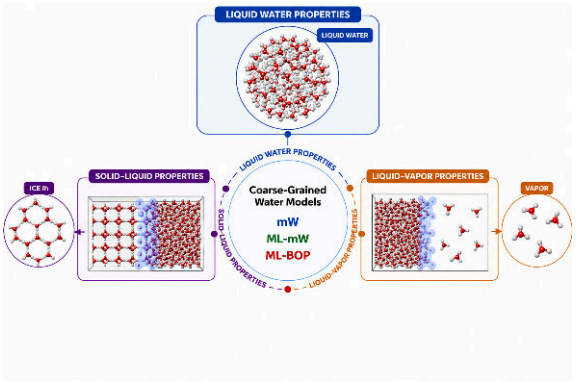



**Figure 1.** Overview of the coarse-grained water models mW, ML-mW, and ML-BOP and their representation of key liquid-water, solid–liquid, and liquid–vapor properties.

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**Keywords:** Coarse-grained water models; structural responsiveness; model transferability; water anomalies

# Decoding the Rate Determining Step in *plasmidium* SHMT to Guide Antimalarial Inhibition:A QM/MM Enhanced-Sampling Free-Energy Study

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Malaria continues to cause over 200 million infections and roughly 450,000 deaths annually, and the spread of drug-resistant *Plasmodium* strains has eroded the efficacy of classical antifolates targeting dihydrofolate reductase and dihydropteroate synthase. In the recent years, serine hydroxymethyltransferase (SHMT) has emerged as a potential next-generation antimalarial target. Motivated by this, we investigate the mechanism of the folate cycle involving SHMT to identify potential targets for inhibitor design. Here we focus on the step involving retro-aldol C$\alpha$–C$\beta$ cleavage of the serine external aldimine. We employ a combination of hybrid QM/MM and enhanced sampling molecular dynamics approaches to decipher the mechanism and to compute free energy barriers along potential reaction pathways. Based on these results, we report the preferred pathway for the reaction.

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**Keywords:** SHMT; QM/MM; free-energy simulation; antimalarial drug target; PLP tautomerism

# Disentangling Heterogeneous Trajectory Ensembles by an Automated and Explainable Framework for Pathway Clustering and CV Identification

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Characterizing complex biomolecular processes—such as protein conformational transitions and ligand unbinding—requires disentangling distinct transition mechanisms from heterogeneous trajectory ensembles. Conventional dimensionality reduction methods treat each frame independently, discarding the temporal ordering and path geometry that define complete molecular transitions. Here, we introduce an automated framework that treats reactive trajectories as single objects and directly compares, embeds, and clusters them into a low-dimensional space. Our method substantially generalizes Functional Diffusion Maps (FDM) [1] beyond its original formulation for scalar functional data, to high-dimensional molecular transitions with heterogeneous temporal sampling, duration, and path geometry. By normalizing time to a common scale and applying geometric distance metrics [2,3], we measure the similarity of two pathways independently of how fast or slowly each transition occurs. These path similarities define the transition probability matrix of a random walk across trajectory space, whose leading eigenvectors project mechanistically related pathways into a low-dimensional map where similar transitions naturally cluster. To translate these abstract diffusion coordinates back into physical mechanisms, we use tree-based models and SHAP feature attribution to connect embedding coordinates to trajectory-level statistical features (such as running averages, fluctuations, and structural deviations) and identify the specific molecular interactions and geometric variables that drive pathways to diverge. We validate FDM across diverse benchmark systems, including alanine dipeptide isomerizations ($\alpha_R$ vs. $\alpha_L$), host–guest unbinding pathways (wet vs. dry routes), and adenylate kinase (AdK) open-to-closed transitions generated by multiple distinct path-sampling algorithms. In each case, FDM accurately separates competing transition mechanisms, while SHAP attribution pinpoints the critical physical collective variables responsible for pathway divergence and bifurcations. This approach provides an automated, interpretable pipeline for discovering reaction pathways and decoding the molecular mechanisms governing complex biomolecular dynamics.

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**Keywords:** Molecular dynamics; Path clustering; Dimensionality reduction; Collective variable identification; Explainable machine learning

# Mechanistic Insights into Substrate Recognition by the Key Quorum-Sensing Regulator Protein SepM in *Streptococcus mutans*

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In *Streptococcus mutans*, the extracellular protease SepM cleaves the 21-residue precursor (21-CSP) into active 18-CSP, initiating biofilm formation vital for dental caries. The mechanisms of how SepM recognises and cleaves 21-CSP are not fully understood. Using an integrated approach combining experimental data, computational techniques, and free-energy calculations, we explored the structural and energetic basis of 21-CSP recognition. We examined how residue interactions and conformational changes affect the formation of a productive 21-CSP: SepM complex necessary for catalysis. Binding of 21-CSP to SepM caused a conformational shift in 21-CSP from unstructured to a coil-helix-coil form and changed the protonation state of Sepm's catalytic lysine from uncharged to charged. A previously unknown region at Sepm's N-terminus forms a hydrophobic patch that accommodates 21-CSP's hydrophobic residues. Free-energy simulations estimated the contribution of eight 21-CSP residues to SepM binding; F11 and N12 contribute most, each over 3 kcal/mol, while L4, F7, L10, and F15 contribute 1- 2 kcal/mol. Mutations in 21-CSP (except L10A and L19A) tend to destabilise non-productive conformations, impeding catalysis, clarifying prior alanine-scanning results. The study links thermodynamic data with structural insights, filling gaps in understanding 21-CSP processing by SepM in *S. mutans*. (*Manuscript submitted*)

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**Keywords:** Free energy calculations, Catalysis, Molecular dynamics, alanine scanning

# Implicating the Role of Enhanced Oxyl Attribute in Facilitating Exceptional C-H Activation by a $[Co^{III,IV}_2(\mu\text{-}O)_2]$ Diamond-Core Complex: A Theoretical Perspective

Rahul Sutradhar[1], Ishita Bhattacharjee[1], Ankan Paul*[1]

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C-H activation is a key biochemical process often facilitated by heme and nonheme enzymes through high-valent metal-oxo species. Among these, nonheme di-nuclear iron-dependent enzyme, soluble methane monooxygenase (sMMO), stands out for its ability to activate strong C-H bonds via a diiron(IV) intermediate[1]. Our study focuses on a cobalt diamond core complex $[Co^{III,IV}_2(\mu\text{-}O)_2]$ supported by a tris(2-pyridylmethyl)amine(TPA) ligand, which has been experimentally proven to have a remarkably high rate constant for C-H bond activation in 9,10-dihydroanthracene(DHA), surpassing analogous first-row transition metal complexes, including the well-established diiron systems[2]. Employing Broken Symmetry Density Functional Theory (BS-DFT) and Complete Active Space Self-Consistent Field (CASSCF) methods, we have theoretically investigated the mechanistic pathways through the prism of multi-state reactivity and unearthed the electronic factors driving such C-H activation process.[3] Comparative barrier analyses between cobalt and iron diamond core complexes further reveal the distinctive advantages of the cobalt system in understanding metal-oxo mediated hydrogen abstraction.

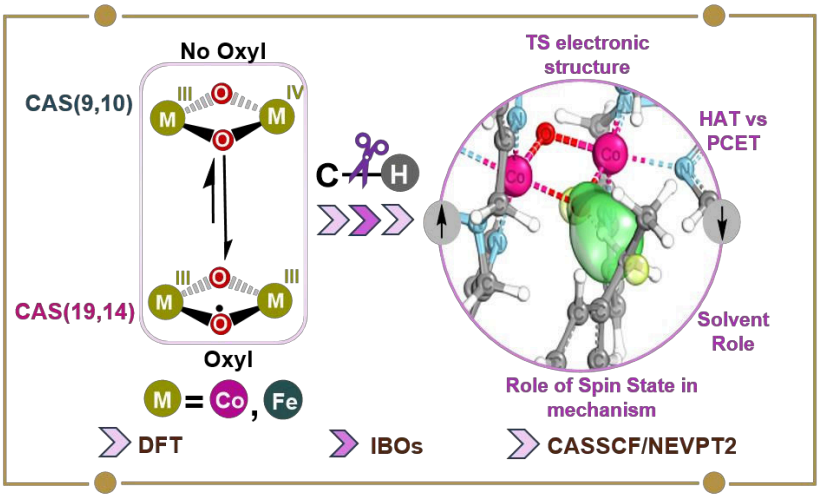



**Figure 1.** Schematic representation of the work.

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**Keywords:** BS-DFT; Electronic Structure; CASSCF/NEVPT2, HAT vs PCET; Solvent Role

# Synthesis and Characterization Study of Precursor-Controlled Multicolour Carbon Quantum Dots for Bioimaging and Drug Delivery Applications

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Fluorescent Carbon Quantum Dots (CQDs) continue to attract attention in nanomedicine because of their tunable emission, aqueous compatibility, negligible toxicity, and surface modification compared to conventional heavy-metal-based quantum dots [1,2]. In this work, a single precursor, O-phenylenediamine, was used to synthesized CQDs of different emission colors simply by changing the oxidant and reaction conditions. Using $H_2O_2$ as the oxidizing agent yielding CQDs with a green emission, whereas replacing $H_2O_2$ with $H_2SO_4$ and introducing ethylenediamine as a co-reactant produced CQDs with a red shifted emission [3,4]. Both CQDs were characterized in detail, including UV-Vis absorption, steady-state photoluminescence, excitation-emission matrix (EEM) mapping, FTIR, along with additional structural and optical characterization. The green-emissive CQDs showed a clear emission maximum around 570 nm under 405 nm excitation. While the red-emissive CQDs displayed multiple excitation-dependent emission bands extending up to 620 nm, indicating that the same core precursor can be pushed toward distinct optical outputs purely through reaction conditions. Surface functional groups identified via FTIR point toward amine- and oxygen-rich passivation contributing to the observed emission behavior [4]. Blue-emissive CQDs are currently being synthesized to complete a multicolor set derived from this single precursor. The resulting CQDs will subsequently be evaluated for cellular uptake and bioimaging via confocal microscopy, along with drug-loading and release studies to assess their potential as nanocarriers [1,2]. This precursor-based, condition-tunable strategy offers a simple route toward multicolor CQDs with dual potential in bioimaging and targeted drug delivery.

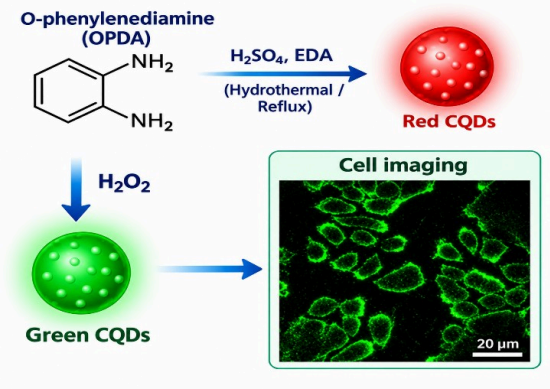



**Figure 1.** Graphical representation of Synthesis of CQDs and cell imaging.

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**Keywords:** Carbon quantum dots, Drug delivery, Precursor-controlled synthesis, Multicolor photoluminescence, Confocal microscopy.

# Engineering Nanoscale Interfaces for Enhanced Förster Resonance Energy Transfer

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Enhancing Förster resonance energy transfer (FRET) in semiconductor quantum dot (QD) assemblies is crucial for advancing optoelectronic, sensing, bioimaging and nanophotonic technologies.[1-2] Herein, we demonstrate an interfacial engineering strategy employing cetyltrimethylammonium bromide (CTAB) and ZnS quantum dots (QDs) to regulate nanoscale energy transfer in CdS and zinc quinolate complex (ZQC)-based donor–acceptor systems.[1-2] In $CdQ_2$-attached CdS QD–Rhodamine B (RhB) assemblies, CTAB effectively passivates surface trap states while reducing donor–acceptor separation through electrostatic anchoring and hydrophobic association.[1] Structural, spectroscopic, zeta-potential and time-resolved photoluminescence analyses confirm enhanced photophysical properties and nearly two-fold improvement in FRET efficiency from 35.8 to 71.3%.[1] In a complementary ZQC-RhB system, CTAB increases FRET efficiency from 13.1% to 49%, while the synergistic incorporation of ZnS QDs further boosts energy transfer to an exceptional 93.6%.[2] NMR, FTIR and density functional theory calculations elucidate the molecular interactions, electronic coupling and interfacial structural changes responsible for this enhancement.[1-2] These findings establish surfactant-assisted QD engineering as an effective strategy for controlling energy transfer, providing a versatile platform for next-generation lighting, sensing, bioimaging, optoelectronics and nanophotonics.

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**Keywords:** Förster Resonance Energy Transfer (FRET); Quantum Dots; Interfacial Engineering; Cetyltrimethylammonium Bromide (CTAB); Rhodamine B

# Self-Assembled PTCDA Coatings on Graphene Profoundly Improve the Biocompatibility Toward Genetic Materials

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In recent years, graphene and other two-dimensional (2D) materials have garnered tremendous research attention in bio-nanomedicine. Nevertheless, their successful application has been plagued by severe nanotoxicity, particularly towards genetic materials, arising from strong non-covalent van der Waals and π–π stacking interactions between the aromatic material surfaces and DNA nucleobases. [1, 2] Herein, using in silico methods based on density functional theory (DFT) and classical molecular dynamics (MD), we propose a biocompatible coating strategy for graphene using perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA), in which the coated heterostructures preserve the structural integrity of double-stranded DNA (dsDNA). PTCDA molecules adsorb flat on graphene through π–π stacking and form self-assembled ordered monolayers and bilayers at temperatures of 500 K and above via van der Waals epitaxy. On uncoated graphene, the dsDNA is severely damaged through the gradual loss of inter-strand Watson-Crick H-bonding and intra-strand π-π stacking interactions. In contrast, graphene coated with a bilayer of PTCDA molecules completely preserves the structure of dsDNA, while the monolayer-PTCDA coating can slightly disturb the terminal nucleobase pairs only. The enhanced biocompatibility of the coating stems from the dual role of PTCDA: first, as a flat aromatic molecule, it can form a layer-by-layer coating on graphene through π-π stacking, thereby making the coating thermally stable due to its polar nature and creating a barrier between graphene and the biomolecule. Secondly, the PTCDA coating interacts with DNA primarily through H-bonds and electrostatic interactions, while van der Waals interactions play second fiddle. The reduced strength of van der Waals interactions and the absence of direct π-π stacking between the nucleobases and graphene upon coating prevent structural damage to DNA. Electronic structure calculations clearly rule out any possibility of chemical reactions between DNA and PTCDA, a sine qua non for biocompatible coatings. The relative biocompatibilities of the monolayer and bilayer PTCDA-coated graphene were estimated to be 78% and 93%, respectively, compared to pristine graphene [3]. PTCDA bilayer-coated graphene is further shown to release a dsDNA within a therapeutically meaningful timescale, unlike pristine graphene. These findings establish PTCDA coating of graphene as an effective method for fabricating low-dimensional, biocompatible heterostructures by efficient screening noncovalent interactions.

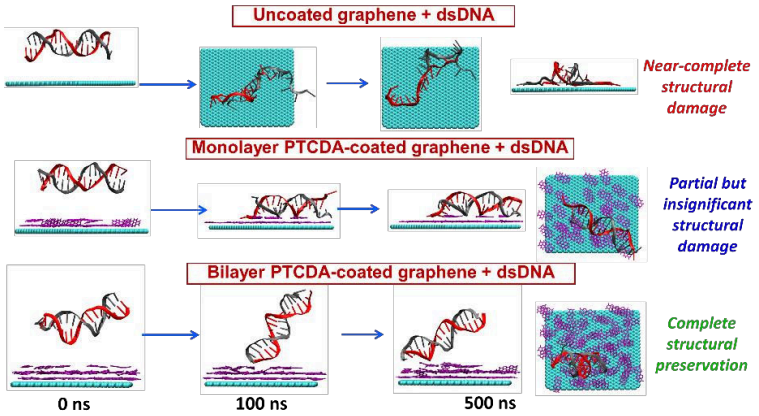



**Figure 1.** Adsorption of dsDNA on uncoated, monolayer-, and bilayer-PTCDA-coated graphene, illustrating coverage-dependent changes in DNA adsorption and structural integrity.

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**Keywords:** Bio-nanotechnology; nanotoxicity; biocompatible coating; graphene; two-dimensional materials; molecular dynamics; density functional theory; non-covalent interactions; free energy calculations.

# Precise Control of Charge-Transfer for Triplet Harvesting: Functional Molecular Designs for High-Efficiency Narrowband TADF-OLEDs

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Keywords: Hyperfluorescence, Multiresonance, Charge-Transfer, Exciplex, TADF-OLED

A central challenge in organic optoelectronics is the inefficient utilization of non-emissive triplet excitons, which limits the internal quantum efficiency of purely organic materials to 25%. Rational charge transfer in donor-acceptor (D-A) molecular designs enables thermal up-conversion of triplet excitons into emissive singlet states, achieving nearly 100% internal quantum efficiency through thermally activated delayed fluorescence (TADF) and room-temperature phosphorescence (RTP). These approaches provide viable, environmentally benign alternatives to expensive, toxic, heavy-metal-based phosphors and are directly relevant to next-generation OLED technologies.

Subsequently, incorporating main-group boron elements into nano-graphene-type polycyclic aromatic hydrocarbon frameworks to achieve multi-resonance paved the way for designing novel TADF emitters with near-unity quantum efficiency. This presentation includes advanced ultrafast photophysics, device physics, exciplex OLEDs, and hyperfluorescence OLED technologies, bridging molecular design and device engineering.

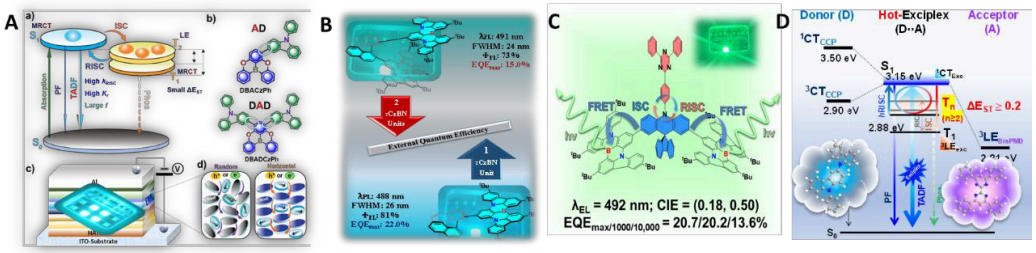



**Figure 1:** A) MRCT-TADF, B) BINAP-locked MR-TADF, C) MR-TADF Dendrimer, D) Exciplex TADF.

**Acknowledgments**: JSPS, Kyulux, OPERA, Kyushu University

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