

Frontiers of Physical Chemistry (FPC 2026): Experiments, Computations and Theory

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

SBO / MCO: Named Oration Lecture, 30 minutes (25+5)

EL: Special Evening Lecture, 60 minutes (45+15); all three are delivered online

IL: Invited Lecture, 20 minutes (17+3)

SL: Invited Lecture (short format), 15 minutes (12+3)

IP: Invited Faculty Poster · P: Contributed Poster · SP: Sponsor Talk, 10 minutes

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) <i>Is the distance between two atoms enough to conclude about bonding?</i>
09:35 – 09:55	IL-02	Sarika Maitra Bhattacharyya (CSIR-NCL Pune) <i>Beyond Crystallization Frustration: Structure and Dynamics in Model Glass Former</i>
09:55 – 10:15	IL-03	Pradipta Bandyopadhyay (JNU New Delhi) <i>Generalizing Physics-based Machine Learning for prediction of hydration free energies</i>
10:15 – 10:30	SL-01	Srestha Basu (SINP Kolkata) <i>Engineering Chemical Reactivity and Optical Response through Defect Design in Nanocluster Assemblies</i>
10:30 – 11:00		Tea Break
SESSION 2 (Chair: Sumana Dutta (IIT Guwahati))		
11:00 – 11:20	IL-04	Moloy Sarkar (NISER Bhubaneswar) <i>From Surface Chemistry to Excited-State Reactivity: Unraveling Catalysis in Mono- and Bimetallic Nanoclusters</i>
11:20 – 11:40	IL-05	Durba Roy (BITS Pilani, Hyderabad) <i>What Nonequilibrium Work Theorems Tell Us About Carbohydrate Mechanics</i>
11:40 – 12:00	IL-06	Partha Hazra (IISER Pune) <i>TADF-Enabled Triplet Exciton Harvesting in Novel Organic Multi-functional Luminogens</i>
12:00 – 12:20	IL-07	Ankan Paul (IACS Kolkata) <i>Shedding Light on the Mechanism of Highly Selective Toluene Photo-oxidation under Nano-Confinement</i>
12:20 – 12:35	SL-02	Saumyak Mukherjee (IISER Berhampur) <i>A Bayesian Lens on Molecular Rigidity: Learning Atomic Weights from Ensemble Data</i>
12:35 – 12:45	SP-1	Sponsor Talk
12:45 – 14:00		Lunch
SESSION 3 (Chair: Pratim Chattaraj (SNBNCBS Kolkata))		
14:00 – 14:20	IL-08	Snehasis Daschakraborty (IIT Patna) <i>CO₂ Adsorption in Humid COFs: A Transition Matrix Monte Carlo Study</i>
14:20 – 14:40	IL-09	Ayan Datta (IACS Kolkata) <i>Buckling and Defects in Two-Dimensional Atomically Thin Monolayers</i>
14:40 – 15:00	IL-10	Debashis Barik (University of Hyderabad) <i>Power-law scaling of depth of the potential wells in bistable systems</i>
15:00 – 15:15	SL-03	Supratik Sen Mojumdar (IIT Palakkad) <i>Small-Molecule-Directed Self-Assembly of Amino Acids for Emergent Fluorescence</i>
15:15 – 15:45		Tea Break
SESSION 4 (Chair: Rajarshi Chakrabarti (IIT Bombay))		
15:45 – 16:05	IL-11	Srabani Taraphder (IIT Kharagpur) <i>Free Energy and Kinetics of Unbinding of Enzyme Inhibitors</i>

16:05 – 16:25	IL-12	Debasis Koley (IISER Kolkata) <i>In Silico mechanistic rationalization of Copper-complex catalyzed oxidative reactions</i>
16:25 – 16:40	SL-04	T. Rajagopala Rao (IIT Patna) <i>Quantum Nuclear Dynamics: Reactive Scattering and Vibronic Coupling</i>
SESSION 5 — POSTER SESSION A (Chair: Surajit Maity (IIT Hyderabad))		
16:45 – 18:15		<i>Invited faculty posters IP-01 to IP-07 Contributed posters P-001 to P-036</i>
18:15 – 18:30		<i>Break</i>
SESSION 6 — SPECIAL EVENING LECTURE (online) (Chair: Anindya Datta (INST Mohali))		
18:30 – 19:30	EL-1	Biman Bagchi (IISc Bengaluru) — online <i>From Molecular Chirality to Living Helices: Symmetry Breaking, Cooperativity, and Handedness Selection</i>
19:30		<i>Dinner (SNBNCBS)</i>

DAY 2 — Thursday, 29 October 2026

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

14:45 – 15:00	SL-11	Debasish Mondal (IIT Tirupati) <i>Reset Controlled Non-equilibrium Transition in an Inhomogeneous Brownian Information Engine</i>
15:00 – 15:15	SL-12	Somrita Ray (IISER Berhampur) <i>Stochastic Resetting Prevails Over Sharp Restart for Broad Target Distributions</i>
SESSION 10 (Chair: Sabyashachi Mishra (IIT Kharagpur))		
15:15 – 15:35	IL-19	Varadharajan Srinivasan (IISER Bhopal) <i>An analytical hydrodynamic model for coupled edge plasmons in TMD nanoflakes</i>
15:35 – 15:55	IL-20	Himansu Sekhar Biswal (NISER Bhubaneswar) <i>From Conformer Resolution to Bond Scission: An Integrated Approach Using REMPI, RIDIR, and VCD/ECD Spectroscopy</i>
15:55 – 16:15	IL-21	Sanjoy Bandyopadhyay (IIT Kharagpur) <i>Modified Interfacial Environment around Biomolecules in Aqueous Ionic Liquid Mixtures</i>
SESSION 11 — POSTER SESSION B (Chair: Soumen Ghosh (IISc Bengaluru))		
16:15 – 17:45		<i>Invited faculty posters IP-08 to IP-17 Contributed posters P-037 to P-069</i>
17:45 – 18:00		<i>Break</i>
SESSION 12 — SPECIAL EVENING LECTURE (online) (Chair: Amalendu Chandra (IIT Kanpur))		
18:00 – 19:00	EL-2	Sudipta Maiti (BITS Pilani, Hyderabad) — online <i>Deep tech in photonics needs talent, ideas, resources, AND deep experience: let's put them together</i>
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 Tapas Chakraborty (MAKAUT, West Bengal) <i>Mass Spectrometry in Physical Chemistry Research</i>
09:30 – 09:50	IL-22	Rajesh Murarka (IISER Bhopal) <i>Understanding the coil-globule transition in semi-flexible polymers from an energy landscape perspective</i>
09:50 – 10:10	IL-23	Ranganathan Subramanian (IIT Patna) <i>Atmospheric Oxidation Kinetics of Emerging Halogenated Oxygenated Volatile Organic Compounds (XOVOCs)</i>
10:10 – 10:30	IL-24	Anirban Misra (University of North Bengal) <i>Theoretical Design and Electronic-Structure Engineering of Donor–Acceptor π-Conjugated Molecular Systems for Tunable Nonlinear Optical Properties</i>
10:30 – 11:00		<i>Tea Break</i>
SESSION 14 (Chair: V. Subramanian (SRMIST Chennai))		
11:00 – 11:20	IL-25	Mousumi Das (IISER Kolkata) <i>Role of excited states in optoelectronics: A model exact and DMRG study</i>
11:20 – 11:40	IL-26	Hemant Kumar Kashyap (IIT Delhi) <i>Insights Into Antibacterial Action of Transition Metal Dichalcogenides</i>
11:40 – 12:00	IL-27	Tushar Debnath (Shiv Nadar University) <i>Exciton-Plasmon Coupling in Plasmonic Perovskite Nanocrystals</i>
12:00 – 12:20	IL-28	Sanjib Senapati (IIT Madras) <i>Reinventing the Drug Formulation Technology for Improved Onset of Action and Lower Dose Requirements</i>
12:20 – 12:35	SL-13	Arnab Halder (Presidency University, Kolkata) <i>Role of Photoinduced Processes to Modulate the Optical Properties of Carbon Nanoparticles</i>
12:35 – 12:45	SP-2	Sponsor Talk
12:45 – 14:00		<i>Lunch</i>

SESSION 15 (Chair: Sanjib Bagchi (RKM Vivekananda Centenary College, Rahara))		
14:00 – 14:20	IL-29	Biman Jana (IACS Kolkata) <i>Learning Transferable Collective Variables For Ligand Binding Transition Through Explainable Machine Learning</i>
14:20 – 14:40	IL-30	Manik Pradhan (SNBNCBS Kolkata) <i>Cavity Ring-down Spectroscopy in Gas and Condensed Phases</i>
14:40 – 14:55	SL-14	Tatini Rakshit (Shiv Nadar University) <i>Probing cancer biomarkers using a biophysical approach</i>
14:55 – 15:10	SL-15	Tapta Kanchan Roy (University of Delhi) <i>An Efficient Variational Approach for Thermal Density Matrices with Quantum Anharmonic Effects</i>
15:10 – 15:25	SL-16	Atanu Singha Roy (NIT Meghalaya) <i>Protein Corona Modulated Doxorubicin Loading and Release from Catechin-Functionalized Ag–Au Alloy Nanoparticles</i>
15:25 – 15:45		<i>Tea Break</i>
SESSION 16 (Chair: Avisek Das (IACS Kolkata))		
15:45 – 16:00	SL-17	Samiran Sen (Institut Pasteur, Paris) <i>Learning what to trust: A Bayesian framework for protein model refinement</i>
16:00 – 16:15	SL-18	Brindaban Modak (BARC Mumbai) <i>Density Functional Theory Study of Single-Atom Catalysts on Porphyrin-like Porous Fullerene for Energy Applications</i>
16:15 – 16:30	SL-19	Anupam Bera (University of Hyderabad) <i>Molecular Structure and Ultrafast Charge-Transfer Dynamics at Functional Material Interfaces: Insights from VSFG and Transient Absorption Spectroscopy</i>
16:30 – 16:45	SL-20	Suman Das (GITAM University, Visakhapatnam) <i>Proteins in Deep Eutectic Solvents: Molecular Insights from Simulations</i>
SESSION 17 — POSTER SESSION C (Chair: Debabrata Seth (IIT Patna))		
16:45 – 18:15		<i>Invited faculty posters IP-18 to IP-26 Contributed posters P-070 to P-103</i>
18:15 – 18:30		<i>Break</i>
SESSION 18 — SPECIAL EVENING LECTURE (online) (Chair: Ranjit Biswas (SNBNCBS Kolkata))		
18:30 – 19:30	EL-3	Mark Maroncelli (Penn State University, USA) — online <i>Adventures of a Lonely Water Molecule as Told by IR, FIR, NMR Spectroscopy and MD Simulation</i>
19:30		<i>Dinner (SNBNCBS)</i>

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) <i>Thermophysical and dynamical properties of liquid sodium: Insights from MD simulations and DFT-BTE theory</i>
09:20 – 09:40	IL-32	Sayan Bagchi (CSIR-NCL Pune) <i>Water Dynamics in Biomolecular Condensates: Beyond Slow Biomolecular Diffusion</i>
09:40 – 10:00	IL-33	Milan Hazra (IIT Jodhpur) <i>Decoding Molecular Grammar of Heterotypic Biomolecular Condensates: Interplay of Sequence Architecture and RNA-like polyelectrolyte Mediated Competitive Interactions</i>
10:00 – 10:15	SL-21	Biswajit Guchhait (Shiv Nadar University) <i>Domain-Specific Dynamics and Solvent-Controlled Excited-State Proton Transfer in Deep Eutectic Solvents</i>
10:15 – 10:30	SL-22	Rakesh S. Singh (IISER Tirupati) <i>From Interactions to Architecture: Rational Design of Biomolecular Condensate Morphologies</i>
10:30 – 11:00		<i>Tea Break</i>

SESSION 20 (Chair: Chaitali Mukhopadhyay (University of Calcutta))		
11:00 – 11:20	IL-34	Pradipta Purkayastha (IISER Kolkata) <i>Epitaxial Assembly of 1D/2D Organic Lateral Heterojunctions for Integrated Photonics</i>
11:20 – 11:40	IL-35	Rahul Sharma (St. Xavier's College (Autonomous), Kolkata) <i>Transient collective motion and density voids in a model drying chemotactic bacterial film</i>
11:40 – 11:55	SL-23	Satyapriya Bhandari (Kandi Raj College) <i>Engineered Nanoarchitectures for Enhanced Energy Transfer and Multifunctional Applications</i>
11:55 – 12:10	SL-24	Piyush Mishra (IIT Kharagpur) <i>Understanding Chemical Mechanisms Through Molecular Spectroscopy</i>
12:10 – 12:20	SP-3	Sponsor Talk
12:30 – 13:00		Valedictory Session
13:00 – 14:00		<i>Lunch and departure</i>

POSTER PRESENTATIONS

POSTER SESSION A — Day 1, Wednesday 28 October 2026, 16:45 – 18:15 (Session 5)

No.	Presenter	Affiliation	Title
IP-01	Bidyut Sarkar	Shiv Nadar University	Investigation of conformational dynamics and ligand binding mechanism of gene regulatory SAM-II / SAM-V tandem riboswitch
IP-02	Niladri Patra	IIT (ISM) Dhanbad	Mapping Conformational and Kinetic Landscapes of 14-3-3 σ / α -Synuclein Assembly via Variational Autoencoders and Markov State Models
IP-03	Saumyak Mukherjee	IISER Berhampur	A Bayesian Lens on Molecular Rigidity: Learning Atomic Weights from Ensemble Data
IP-04	Debdas Dhabal	IIT Guwahati	CMA-ES-based Force Field Parameter Optimization of Diiodomethane for Surface Free Energy Calculations
IP-05	Pradip K. Ghorai	IISER Kolkata	Breaking Azeotropes: The Role of Entrainers in Efficient Separation
IP-06	Papri Chakraborty	IIT Kharagpur	Activation of atomically precise monolayer-protected Pt nanoclusters: Formation of active CO oxidation catalysts
IP-07	Utpal Sarkar	Assam University, Silchar	Machine Learning Approach to Screen Potential Donor and Acceptor Fragments: Insights from Chemical Reactivity
P-001	Hirak Jyoti Baishya	IIT Guwahati	Targeting Plasmodium Falciparum Purine Nucleoside Phosphorylase (PfPNP) with Unnatural Nucleosides: A Computational Study
P-002	Surendra Nath Barman	NIT Meghalaya	BSA Conjugated Carbon Nanotubes for Release of Potent Antioxidant Curcumin
P-003	Keniya Basu	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	IIT Kanpur	Quantum phase transitions in time-dependent quantum mechanical scattering
P-005	Suman Bhowmik	IIT Kanpur	Decoding Intersystem Crossing: Molecular Design, Vibrational Control and Environmental Modulation
P-006	Partha Pratim Borah	IIT Guwahati	Rethinking Activity Descriptors for Single-Atom Iron Water Oxidation Catalysts
P-007	Roohi Choudhury	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	IIT Kanpur	Unraveling the Dynamics of Interfacial Water at Electrified Graphene Surfaces through Theoretical Two-Dimensional Vibrational Sum-Frequency Generation Spectroscopic Study
P-009	Hrishika Dey	IIT (ISM) Dhanbad	Targeting Plasmodium falciparum Calcium-Dependent Protein Kinases: Opportunities for Novel Antimalarial Therapeutics
P-010	Sampriti Ghosh	SINP Kolkata	Lanthanide-Doped Gold Nanocluster Assemblies Exhibiting Dopant-Directed Size Evolution, Symmetry-Controlled Eu ³⁺ Emission, and Selective Chemical Recognition
P-011	Mansi Gupta	Shiv Nadar University, Delhi-NCR	Ultrafast Hole Transport via Host–Guest Binding in Perovskite Nanocrystals: Experiment and Theory
P-012	Injamamul Haque	Presidency University, Kolkata	Tuning Hydrogen Abstraction Reactivity of Fe(IV)=O Corrole Complexes through Local Electric Fields
P-013	Krishna	SVNIT Surat	Interaction Mechanism in LiH-nNH ₃ BH ₃ (n=1-2) Complexes: Insights from Vibrational and Chemical

No.	Presenter	Affiliation	Title
			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	IISER Kolkata	Unravelling Magnesium Dependent Conformational Switching in Flaviviral RNA
P-016	Sankar Maity	NIT Rourkela	Glucose-Mediated Stabilization of Ethanol-Stressed Lipid Bilayers: Insights from Molecular Dynamics
P-017	Srimila Mallick	IIT Guwahati	Enhanced Inhibition of Amyloid β Oligomerisation by a Coumarin- Chalcone Hybrid over a Coumarin Derivative
P-018	Sourav Manna	IIT Kharagpur	Thermal and Light-Induced Catalysis in Pyridoxal 5'-Phosphate-Dependent Aspartate Aminotransferase
P-019	Balaram Mondal	IIT Guwahati	Ligand-Specific Binding Mechanism and Dynamic Modulation of Auxin Receptor TIR1 by Structurally Diverse Auxin Analogs
P-020	Anwesha Mukherjee	University of Kalyani	Bile salt incorporated vesicles – Modulation of their characteristics and fluorescence probing of their microenvironment
P-021	Rik Niranjan Mukherjee	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	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	IIT Kanpur	Dynamical quantum chaos in one-dimensional transverse field Ising model
P-025	Subir Podder	Raiganj University	A Novel Naphthofluorescein Derivative as an Antioxidant for Biodiesel: Integrated DFT, Molecular Dynamics, and Machine Learning Insights
P-026	Priya	IIT Kanpur	Green's function formalism for kinetic energy density functional for atoms.
P-027	Madhumita Rano	Ashoka University, Sonipat	State-specific computations of vibrational and electronic excited states
P-028	Rishu	IIT Delhi	Collective Reaction Dynamics during Ligand Exchange in Atomically Precise Metal Nanoclusters
P-029	Saswata Roy	Azim Premji University, Bengaluru	Challenges in scalable excited state semiclassical dynamics
P-030	Gourab Saha	IACS Kolkata	Quasiclassical Reaction Dynamics: Diels–Alder versus hetero-Diels–Alder Reactions
P-031	Dibyamanjaree Samant	IISER Kolkata	Mapping the sgRNA-induced Cas9 conformational activation pathways integrating structure-based modeling and VAMPnet
P-032	Arka Prava Sarkar	SNBNCBS Kolkata	Investigating the nature of anion migration in halide perovskites in presence of single layer graphene
P-033	Mokshi Sharma	Central University of Jammu	Variational Framework for the Calculation of Vibrational States and Thermal Properties with the Effective Harmonic Oscillator
P-034	Sumit Singha	University of North Bengal	Engineering Nanoscale Interfaces for Enhanced Förster Resonance Energy Transfer
P-035	Ananya Sinha	IACS Kolkata	Accelerating Selected Configuration Interaction with Restricted Boltzmann Machine
P-036	Vishal Yadav	IISER Kolkata	From Cause to Consequence: Explainable AI-Guided

No.	Presenter	Affiliation	Title
			Reaction Coordinate Reveals Thermodynamic and Kinetic Mechanisms of Nucleic Acid Base-Flipping

POSTER SESSION B — Day 2, Thursday 29 October 2026, 16:15 – 17:45 (Session 11)

No.	Presenter	Affiliation	Title
IP-08	Barun Kumar Maity	SINP Kolkata	Specific DNA Recognition Induces Folding Transition of the Oncogenic Fusion Protein PAX3FOXO1
IP-09	Debashree Ghosh	IACS Kolkata	Title to be announced
IP-10	Padmaja Prasad Mishra	SINP Kolkata	Exploring Toehold-Independent DNA Strand Displacement through Parallel Triplex Formation
IP-11	Sudip Das	SINP Kolkata	Physics-Informed Machine Learning for Enzyme Catalysis
IP-12	Amit K. Paul	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	Aliah University, Kolkata	Decoding the Molecular Interactions of Thymol, Thymoquinone, and Lawsone with DNA and Protein: Experimental & Computational Approach
IP-14	Rajarshi Chakrabarti	IIT Bombay	Active Polymers in Porous Media: Activity-Driven Conformational and Transport Dynamics
IP-15	Surajit Maity	IIT Hyderabad	Quantifying the Intrinsic Energetic Thresholds of Solvent-Driven Excited-State Proton Transfer via Isotopic Tunneling Quenching
IP-16	Tushar Kanti Mukherjee	IIT Indore	Regulation of Protease Activity of Papain via Biomolecular Condensation and Its Reactivation by L-Cysteine
IP-17	Arijit Kumar De	IISER Mohali	Unveiling Time-Dependent Vibronic Coupling by Third- and Fifth-order Raman Spectroscopy
P-037	Md Asif Amin	Suri Vidyasagar College	Coronene Based Two Dimensional Metal-Organic Framework with High Spin-Filtering Efficiency
P-038	Nidhi Arya	IIT Jodhpur	Unravelling the Mg ²⁺ -Dependent Structural Dynamics of DNA Holliday Junctions at the Single-Molecule Level
P-039	Indrani Bhattacharya	SNBNCBS Kolkata	Ascorbic Acid Modulates the Hydration Dynamics of Urea and Glucose: Insights from Terahertz Spectroscopy and Molecular Dynamics Simulations
P-040	Sayari Bhattacharya	SNBNCBS Kolkata	The Fibril Tip Sets the Route, Not Just the Destination: Polymorph-Specific Kinetics of A β 42 Monomer Incorporation
P-041	Sakshi Chawla	IIT Gandhinagar	Tailoring Herzberg-Teller Vibronic Interactions in Tetrapyrrole-Based Systems
P-042	Shrestha Chowdhury	SNBNCBS Kolkata	Structural Deviations from Ideality in Alcohol + Water Azeotropes: Molecular Scale Investigations
P-043	Kingshuk Das	IACS Kolkata	Salt-Mediated Molecular Recognition of the p53 C-terminal Domain
P-044	Krishnandu Dey	NIT Meghalaya	Photoswitch activity of an Acyl-hydrazone dimer: A non-adiabatic dynamics study.
P-045	Priya Dey	Kyoto University, Japan	Pepper-Mill Protein Dynamics: Decoding the Mechanism of MSPA for ssDNA Translocation
P-046	Sk Samsul Ghaus	IISER Kolkata	Engineering HLCT-AIE Active Molecule for Efficient Flexible Optical Waveguides: Photophysics, Mechanics, and Optoelectronic Integration
P-047	Oushnik Sen Gupta	SINP Kolkata	Monitoring enzyme activity on the surface of a self-referenced near-white light emitting assembly of

No.	Presenter	Affiliation	Title
			atomic clusters.
P-048	Subhabrata Hazra	IACS Kolkata	Intermediate Relaxation Timescale in Bulk Water: A Temperature-Dependent Investigation
P-049	Tathagata Islam	SINP Kolkata	Supramolecular assembly-driven emergent chirality with simultaneous induction and ligand inversion in atomic clusters
P-050	Vijay Kumar	IIT Kharagpur	Determinant Sampling and Subspace Diagonalization for Strongly Correlated Molecular Systems
P-051	Subrata Kundu	IIT Jodhpur	Mg ²⁺ -Dependent Dynamics and Kinetics of a DNA Holliday Junction Studied by Single-Molecule FRET.
P-052	Himashree Mahanta	Assam Kaziranga University	Chemical Dynamics Simulations of Benzene-Hexachlorobenzene Complexes: Association, Ensuing Dissociation, and Comparison with Related π - π Molecular Complexes
P-053	Koushik Makhal	IIT Hyderabad	A potential gated formic acid oxidation reaction on the Rh-Cr dual-atom catalyst water interface
P-054	Apurba Manna	IIT Kharagpur	Unravelling the Microscopic Properties of a Globular Protein in Aqueous Deep Eutectic Solutions using Molecular Simulations
P-055	Archi Mishra	NIT Karnataka, Surathkal	Effect of membrane composition on the structural dynamics of Amyloid Precursor Protein(APP)
P-056	Piyali Mukherjee	IIT Bombay	A Theoretical Investigation of the Encapsulation of Small Molecules within Coacervates of Elastin-like Polypeptides
P-057	Venkatesh N	IIT Patna	Growth of Low-Density Liquid Domains Drives Fickian, Yet Non-Gaussian Diffusion in Supercooled Water
P-058	Rishabh Kumar Pandey	CUHK Shenzhen	Vibronic Coupling Effects in the Photoelectron Spectra of LiB6-
P-059	Roja Satvika Puvvada	GITAM University	Unravelling the role of aqueous choline chloride-polyol deep eutectic solvents in protein stability
P-060	Rajendra Rath	NIT Rourkela	Emergent Mixed Crowding Effect on Protein Dimerization
P-061	Indranil Roy	IISc Bengaluru	Anisotropic quantum beats report room temperature functional vibronic couplings in light-harvesting aggregates
P-062	Sudhriti Roy	IIT Jodhpur	Engineering Heterotypic Biomolecular Condensates with Synthetic Peptides for Controlled Spatial Organization and Liquid-like Nature
P-063	Gourab Saha	IIT Kharagpur	Molecular Insights into the A β -42 Tetramer Induced Disruptive Effects on a Model Phospholipid Membrane
P-064	Koushik Saha	IACS Kolkata	Quantum Dynamics and Mean Square Displacement of a Nonlinear Brownian Oscillator
P-065	Dipayan Sarder	IIT Kharagpur	Microscopic Understanding of DNA Groove Binding by Hydrophilic and Hydrophobic Ionic Liquids
P-066	Arghya Sen	University of Rostock, Germany	CsMnBr ₃ Nanocrystals: Excitation-Dependent Photophysics and Curious Case of Carrier Dynamics from Picoseconds to Microseconds
P-067	Pallav Sengupta	IIT Guwahati	Distal residue mutations dictate substrate binding in MtbThyX
P-068	Deepak Sharma	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	IISER Pune	Li ₂ O Vacancy-Induced Modulation of Oxygen Redox in Li ₂ MnO ₃ Surfaces: A First Principles Study

POSTER SESSION C — Day 3, Friday 30 October 2026, 16:45 – 18:15 (Session 17)

No.	Presenter	Affiliation	Title
IP-18	Bhabani S. Mallik	IIT Hyderabad	Multiscale Modeling of Electrochemical Catalysis and Energy Storage Systems via Molecular Dynamics Simulations
IP-19	Ranjit Biswas	SNBNCBS Kolkata	Conductivity in Battery Electrolyte Systems: Impact of Ultrafast Solution Dynamics, Ion-Ion Motional Correlations, and Solution Heterogeneity
IP-20	Suman Chakrabarty	SNBNCBS Kolkata	Navigating Pathways in Free Energy Landscape: Adaptive (Machine) Learning Strategies Towards Rare Event Kinetics
IP-21	Souvick Biswas	IISER Thiruvananthapuram	Resonantly Stabilized Free Radical Mediated Mass Growth: Indenyl Chemistry as the Common Thread of Planar and Curved PAHs
IP-22	Anup Ghosh	Bose Institute, Kolkata	Beyond the Sulfoxide Oxygen: NMR Spectroscopy and Machine-Learned Dynamics Reveal α -C-H $\cdots$ Ow Hydrogen Bonding in Dimethyl Sulfoxide-Water
IP-23	Abhijit Dan	MAKAUT, West Bengal	Interfacially Engineered Liquid Crystal Microdroplets: A Robust Platform for Label-Free Optical Biosensing
IP-24	Padmabati Mondal	IISER Tirupati	A multiscale study in search of photoswitchable drug for serotonin receptors
IP-25	Anirban Panda	J. K. College, Purulia	Addition Reaction Networks and Partial Ordering of Phosphorus–Sulfur Binary Compounds: A Theoretical Study
IP-26	Subhadip Ghosh	NISER Bhubaneswar	Spatially Resolved Energy Transfer in Hexagonal Cs ₄ PbBr ₆ Microdisks Revealed by Single-Particle Spectroscopy
P-070	Farhin Akhtar	RGIPT Sivasagar	Multifunctional Plasmonic Fluorescent Nanocomposites for Ultrasensitive Molecular Sensing, Antimicrobial Defense and High Resolution Bioimaging
P-071	Debasish Barman	Kyushu University, Japan	Precise Control of Charge-Transfer for Triplet Harvesting: Functional Molecular Designs for High-Efficiency Narrowband TADF-OLEDs
P-072	Anupaul Baruah	Dibrugarh University	A Light-weight Monte Carlo Simulation Based In Silico Protein Design Method for Mutation Induced Fold Switch
P-073	Sreyan Bhowmick	SNBNCBS Kolkata	Ligand-driven entropic collapse directs mechanical strain to facilitate BirA dimerization
P-074	Ipsita Chakraborty	S. M. College, Bhagalpur	Unravelling PNIPAM Hysteresis: A Solvent Relaxation NMR Study of the Globule-to-Coil Transition
P-075	Samsung Raja Daimari	IIT Guwahati	Gas and Aqueous Phase Oxidation of a Series of Lactones: Initiated with OH Radicals
P-076	Supritam Datta	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	IACS Kolkata	Effect of Protein on Photoisomerization of Bacteriophytochrome
P-078	Parineeta Gogoi	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	IIT Guwahati	Unveiling the Influence of Biomolecules on the Relaxivity of Mn(II) Based Contrast Agents: A Molecular Dynamics Study
P-080	Aanchal Hurmade	IISc Bengaluru	Raman Spectroscopic Investigation of Biochemical

No.	Presenter	Affiliation	Title
			Changes in Imiquimod-Induced Psoriasis Model.
P-081	Mira Jhavar	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	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	IACS Kolkata	Committer-Based Detection of Post-Transition-State Bifurcations from Enhanced-Sampling Simulations
P-084	Dibyendu Maity	SNBNCBS Kolkata	Quantitative Pathway-Resolved Kinetics from Neural Network-Guided Weighted Ensemble Simulations
P-085	Abdul Aziz Mandal	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	IISc Bengaluru	Stochastic Thermodynamics of a Non-Markovian Random Process
P-087	Anandita Mitra	IIT Guwahati	Therapeutic Targeting of Cancer-Associated PKM2 Mutants by Shikonin via Mutation-Induced Pocket Recognition
P-088	Mainak Mukherjee	Sri Sathya Sai Institute of Higher Learning	Computational Investigation of Through-Bond and Through-Space Charge Transfer for Reduced or Inverted Δ EST in TADF Emitters
P-089	Shreya Mukherjee	IIT (ISM) Dhanbad	Estimation of Absolute Protein–DNA Binding Free Energy using Streamlined Geometric Formalism
P-090	Titas Kumar Mukhopadhyay	NIT Jamshedpur	Self-Assembled PTCDA Coatings on Graphene Profoundly Improve the Biocompatibility Toward Genetic Materials
P-091	Somnath Paitandi	IIT Guwahati	Mg-Co-B Chemical Space for Mg-Ion Cathodes: Evolutionary Search, Machine Learning, and Chemical Bonding Analysis
P-092	Shivam Pandey	IACS Kolkata	Turning Heat into Electricity: Driving High ZT through Soft Phonon Engineering
P-093	Juriti Rajbangshi	University of Wisconsin-Madison, USA	Molecular Insights and Predictive Models for Solvent Selection in Lignin Valorization
P-094	Samarth Razdan	IIT Bhilai	Molecular Engineering of Antiaromatic Orangarin-based Sensitizers for High-Performance Dye-Sensitized Solar Cell Applications
P-095	Roshan	IIT Delhi	Interfacial engineering of waste derived Char/VO ₂ composites for stable electrochemical energy storage
P-096	Arnab Roy	IACS Kolkata	Anti-Kasha-Type Spin-Vibronic Dynamics Drive Photoinduced Ni–H Umpolung in Ni-pincer complex
P-097	Debasish Saha	IISER Bhopal	Non-Markovian escape under stochastic resetting
P-098	Adyasa Sahoo	IIT Guwahati	Structural Responsiveness as the Key to Water's Phase Behavior: Lessons from Machine-Learned mW and BOP Models.
P-099	Jagori Sarkar	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	SNBNCBS Kolkata	Disentangling Heterogeneous Trajectory Ensembles by an Automated and Explainable Framework for Pathway Clustering and CV Identification
P-101	Mohd Ayaz Siddique	IIT Guwahati	Mechanistic Insights into Substrate Recognition by the Key Quorum-Sensing Regulator Protein SepM in Streptococcus mutans

No.	Presenter	Affiliation	Title
P-102	Rahul Sutradhar	IACS Kolkata	Implicating the Role of Enhanced Oxyl Attribute in Facilitating Exceptional C–H Activation by a [Co ² III,IV(μ-O) ₂] Diamond-Core Complex: A Theoretical Perspective
P-103	Himanshu K. Tiwary	IIT Jodhpur	Synthesis and Characterization Study of Precursor-Controlled Multicolour Carbon Quantum Dots for Bioimaging and Drug Delivery Applications