Structure and Dynamics of Chemical and Biomolecular Systems

Oct 26-28, 2023

Venue: Outreach Auditorium, IIT Kanpur

Oct 25 (Arrival Day)

7:30 PM	10:00 PM	Dinner	
Oct 26 (Day 1)			
7:30 AM	8:45 AM	Breakfast	
8:45 AM	9:00 AM	**Inauguration**	
Session 1		*Chair: Vinod K. Singh*	
9:00 AM	9:40 AM	Biman Bagchi (PL1)	*Fundamental, time honoured problems of physical Chemistry and physical biology*
9:40 AM	10:05 AM	Keshavamurthy Srihari	*Isomerization in an optical cavity: Lessons from a simple model*
10:05 AM	10:30 AM	Suman Chakrabarty	*Finding Order Parameters / Reaction Coordinates for Complex Molecular Systems and Exploration of Free Energy Landscapes*
10:30 AM	10:55 AM	Ranjit Biswas	*Alcohol-Water binary azeotropes: Dynamically intriguing but structurally mundane?*
10:55 AM	11:20 AM	Tea Break	
Session 2		*Chair: DLVK Prasad*	
11:20 AM	11:45 AM	Sarika Maitra Bhattacharyya	*Is there a structure-dynamics correlation in supercooled liquids, and does it depend on the interaction potential?*
11:45 AM	12:10 PM	Sanjoy Bandyopadhyay	*Effects of Ionic Liquids on the Interfacial Properties of Amino Acids and Proteins*
12:10 PM	12:35 PM	Rajesh Murarka	*Decoding the Functional Dynamics of β-Arrestins Orchestrated by Distinct GPCR Phosphorylation Patterns*
12:35 PM	1:00 PM	Arnab Mukherjee	*Approaching de novo drug design using a combination of physics-based and Machine learning algorithms*
1:00 PM	2:00 PM	Lunch	
Session 3		*Chair: Mainak Sadhukhan*	
2:00 PM	2:40 PM	Yoshitaka Tateyama (PL2)	*Advanced MD Study on Ion Transport in Battery Solid Electrolyte*
2:40 PM	3:05 PM	Snehasis Chowdhuri	*Solvation structure and dynamics of cis- and trans-N-methylformamide*
3:05 PM	3:30 PM	Bhabani Shankar Mallik	*Hybrid Heterosurface-Modulated Two-Dimensional Hydrogen Bond Structure of Water*
3:30 PM	3:55 PM	Photo Session	
3:55 PM	4:20 PM	Tea Break	
Session 4		*Chair: Devendra Mani*	
4:20 PM	4:45 PM	Debashree Chakraborty	*Mechanism of ion permeation in membrane: an insight from MD simulations*
4:45 PM	5:10 PM	Avisek Das	*Correlated disorder in entropic crystals*
5:10 PM	5:20 PM	Netweb	
5:30 PM	7:30 PM	**Poster Presentations - 1**	
7:30 PM	10:00 PM	Dinner	

Oct 27 (Day 2)			
7:30 AM	9:00 AM	Breakfast	
Session 5		*Chair: Debabrata Goswami*	
9:00 AM	9:40 AM	Dominik Marx (PL3)	*Highly Accurate Path Integral Simulations Enabled by Machine Learning: From Cryogenic Solvation to Coupled Cluster Liquid Water*
9:40 AM	10:05 AM	Srikanth Sastry	*The liquid-liquid transition in silicon: Computer simulations and reconstruction of free energy surfaces*
10:05 AM	10:30 AM	Akira Nakayama	*Microscopic Understanding of Interface at Liquid/Solid-Oxide and Molecular Adsorption on the Surface by Neural Network Potentials*
10:30 AM	10:55 AM	Venkat Kapil	*Machine Learning for full quantum first-principles simulations*
10:55 AM	11:20 AM	Tea Break	
Session 6		*Chair: Arnab Ghosh*	
11:20 AM	11:45 AM	Naresh Patwary	*Dynamics of C–C Bond Cleavage: Aromatic vs. Aliphatic Substrates*
11:45 AM	12:10 PM	Satoshi Nihonyanagi	*Molecular-Level Elucidation of Buried Solid/Liquid Interfaces Studied by Heterodyne-detected Vibrational Sum Frequency Generation*
12:10 PM	12:35 PM	Tapas Chakroborty	*Mass-selected Mobility Spectrometry in Molecular Structure Analysis*
12:35 PM	1:00 PM	Sutapa Roy	*Non-equilibrium Dynamics of Fluids upon Temperature Quench*
1:00 PM	2:00 PM	Lunch	
Session 7		*Chair: Vishal G Rao*	
2:00 PM	2:40 PM	Keisuke Tominaga (PL4)	*Dynamics and Structures of Aqueous Solutions and Hydrated Soft Matters Studied by Broadband Dielectric Spectroscopy*
2:40 PM	3:05 PM	Anunay Samanta	*Relaxation Pathways and Dynamics of the Charge Carriers in Perovskite Nanocrystals*
3:05 PM	3:30 PM	Sayan Bagchi	*Probing Nanocrystal Surface Dynamics with 2D IR Spectroscopy*
3:30 PM	3:55 PM	Tea Break	
Session 8		*Chair: Manabendra Chandra*	
3:55 PM	4:20 PM	Elangannan Arunan	*Electron Density as a Probe of Inter- and Intra-Molecular Bonds*
4:20 PM	4:45 PM	Arindam Chowdhury	*Heterogeneous single-molecule transport through a rubbery polymer network*
4:45 PM	5:10 PM	Puneet Gupta	*Boron-based Heterogeneous Catalysts for Methane Oxidation: Catalytic Space, Reactivity and Orbital Analysis*
5:10 PM	5:20 PM	HPE & Savex Technologies	*Sustainable IT Infrastructure Solution for HPC & AI*
5:20 PM	7:00 PM	**Poster Presentations - 2**	
7:30 PM	10:00 PM	**Conference Dinner (Venue: Type 2 Community Center)**	

Oct 28 (Day 3)			
7:30 AM	9:00 AM	Breakfast	
Session 9		*Chair: Sandeep Verma*	
9:00 AM	9:40 AM	Mark Tuckerman (PL5)	*Synergizing enhanced sampling and machine learning strategies in molecular simulation for representing and deploying high-dimensional free energy surfaces and learning reaction coordinates*
9:40 AM	10:05 AM	Srabani Taraphder	*Computer simulation studies on the pH sensitivity of enzyme structure and dynamics*
10:05 AM	10:30 AM	Biman Jana	*Understanding the mechanism of ice nucleation and ice growth inhibition by ice binding proteins (IBPs)*
10:30 AM	10:55 AM	Jagannath Mondal	*Understanding Biomolecular Simulation using Machine-learning*
10:55 AM	11:20 AM	Tea Break	
Session 10		*Chair: J N Moorthy*	
11:20 AM	11:45 AM	R. Sankararamakrishnan	*Non-covalent interactions in the structure, stability and dynamics of biomolecules and biomolecular recognition*
11:45 AM	12:10 PM	Nilashis Nandi	*Unbinding of Non-cognate Antifungal Molecule from the Active Site of Eukaryotic Isoleucyl tRNA Synthetase from Candida Albicans*
12:10 PM	12:35 PM	Susmita Roy	*Tracking the Sequence and Structural Evolution of SARS-CoV-2 Spike Protein*
12:35 PM	1:00 PM	Pradipta Bandyopadhyay	*A fast statistical mechanical model to study solvation in water: Crustwater*
1:00 PM	2:00 PM	Lunch Break	
Session 11		*Chair: Vivek Yadav*	
2:00 PM	2:25 PM	Joseph Brock	*Structural basis of multi-drug resistance in Candida albicans via the transporter CaCDR1*
2:25 PM	2:40 PM	Bikramjit Sharma	*Advancing the Frontier of Electronic Methods for Accurate Computation of EPR Observables in Solution*
2:40 PM	2:55 PM	Banshi Das	*Theoretical Nonlinear Vibrational Spectroscopy of Water in Slit Pores*
2:55 PM	3:10 PM	Saheb Dutta	*QM/MM Simulation to Study the Reaction Pathways of the Charging Step of Aminoacylation Reaction at the Active site of Class I Leucyl tRNA Synthetase and Class II Aspartyl tRNA Synthetase*
3:10 PM	3:30 PM	Poster Awards	
3:30 PM	4:00 PM	Tea Break	
Session 12		*Chair: Vadapalli Chandrasekhar*	
4:00 PM	4:40 PM	Amalendu Chandra (PL6)	*Nonlinear Vibrational spectroscopy of aqueous solutions and interfaces*
4:40 PM	**6:30 PM**	**Special Session on Prof. Amalendu Chandra's 60th Birthday**	
7:30 PM	10:00 PM	Dinner	
Oct 29 (Departure Day)			
7:30 AM	9:00 AM	Breakfast	