SDCBS23:Posters

Session - 1 (26/10/2023, 05:30PM-07:30PM)

Poster No.	Name	Affiliation	Poster Title
1	Yuki Fuji	Kobe University, Japan	Vibrational frequency fluctuations of poly(N,N-diethylacrylamide) at the lower critical solution temperature studied with 2D-IR spectroscopy and MD simulation
2	Vaishali Thakkur	IIT Kanpur	Inhibition Mechanism of Class D β-Lactamases by Avibactam
3	Pranjal Sur	IISc Bangalore	Single Amino Acid Translocation through Graphene Nanopore and Orientation Dependence of Relative Current Blockades.
4	Bijaya Pathak	IIT Bombay	Role of solitary ammonia in proton transfer reactions in weaker acid
5	Saikat Dhibar	IACS Kolkata	Characterizing free energy landscape of flexible polymer chains and small proteins usingoptimized collective variable from Time-Structured Independent Component Analysis and Neural Network
6	Sangita Mondal	IISc Bangalore	Exploring Anomalous Ion Diffusion in Water-DMSO Binary mixture
7	Samprita Nandi	USC, USA	Effect of backbone discontinuity on charge transport in double-stranded DNA
8	Susmita Sarkar	TIFR Hyderabad	Key to Inhibit Pathological Aggregation: Protein Conformational Modification by ATP
9	Soumyadip saha	IIT Kanpur	Kinetic Monte Carlo simulations of m-plane {1-100} GaN thin films
10	Bharath Raj P	IIT Madras	To understand the lipid transfer mechanism and dynamics of CETP bound to different neutral lipids through molecular dynamics simulations
11	Madhusmita Devi	IIT Guwahati	Elucidating the Inhibitory Effect of Whitlock's Caffeine-Pincered Molecular Tweezer on α-Synuclein Aggregation
12	Deepika	IIT Kanpur	Structure and dynamics of Aqueous NaOH Solution using Neural Network Potential
13	Soumik Bardhan	Jadavpur University	How Selected Protic Ionic Liquids Make the Water-in-Oil Microemulsions Proactive: Measurements and Mechanism
14	Prasun Pal	IACS Kolkata	Molecular mechanism of ice nucleation or growth inhibition by ice binding proteins.
15	Projesh Kumar Roy	IIT Madras	Investigation of the co-aggregation mechanism of oncogenic mutant p53 and wild-type p73 tumor suppressor proteins in human cancer cells using computational tools
16	Ashish Kumar	IISER Pune	Spatially-Resolved Analysis of Individual Water Entropy near Amino Acids
17	Pooja Nanavare	IIT Bombay	Dynamics of a methane hydrophobe in aqueous choline chloride solution: Insights from molecular dynamics simulations
18	Hero Khan PATHAN	ITM University	Experimental, computational approaches, Molecular Docking and Molecular dynamic simulation of 4-Amino-3-hydroxy Naphthalene-1-Sulfonic Acid (ANSA)
19	Shivani Verma	IIT Kanpur	A Comprehensive Study of Factors Affecting the Prediction of pKa Shift of Aspartate in Thioredoxin Protein
20	Sangeeta Das	IACS Kolkata	Understanding Molecular Self-assembly via Multidimensional Clustering in the Chemical Interaction Space

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21	Kakali Baruah	NIT Meghalaya	Formation of protein-corona by turmeric and curcumin functionalized AuNPs and human serum albumin (HSA): A detailed investigation into the binding of AuNPs with HSA using spectroscopic and molecular dynamics simulation studies
22	Dulal Mondal	IIT Kharagpur	pH dependent structure and dynamics of human carbonic anhydrase II
23	Dibyendu Mondal	IISc Bangalore	Ion-mediated folding of SMK-box riboswitch
24	Sipra Mohapatra	IIT Jodhpur	How Does Pectin Influence Ion Transport in Liquid Electrolytes?
25	Bikirna Roy	IISER Pune	Interplay of Internal Friction and Memory Effects in Viscosity Dependence of Rates
26	Jyoti Yadav	SLIET	Solvent effect on the excited state dynamics in large stokes-shifted fluorescent benzothiazoles
27	Bhavana Panthi	IIT Kanpur	Free Energy Landscape of the Nucleotide Exchange Mechanism of K-Ras Protein in Presence of its Catalytic Protein SOS
28	Uddipan Bhattacharya	IISER Pune	Finding Potential Lead Molecules for PSMD10 Gankyrin
29	Ravi Malik	IIT Kanpur	Theoretical Vibrational Sum Frequency Generation (VSFG) Spectroscopy of Aqueous Solutions Containing Surfactant Solutes: Effect of Counterions on the Structure and Dynamics of Water
30	SK Habibullah	IISc Bangalore	How Does an RNA Fragment Sense a Metal Ion?
31	Avijit Mainan	IISER Kolkata	Dynamic Counter-ion Condensation (DCC) model captures metal-induced RNA ring threading of SARS-CoV-2 viral RNA
32	D Avinash	IIT Madras	Incorporating Electrostatic complementarity in HIV Protease Inhibitor design to improve binding affinity
33	Deepika Sharma	IIT Kanpur	THz Spectra of Aqueous GdmCl and TMACl Solutions using Molecular Dynamics Simulations with Polarizable Forcefield
34	Shreya Rastogi	IIT Kanpur	Intramolecular Proton Transfer in Pyridoxal 5′-phosphate Schiff Bases and Free Energy Landscape for Transimination Reaction at the Active site of Ornithine Decarboxylase
35	Chinmay Parida	IIT Bhubaneswar	Hydrogen bonding structure and dynamics of water-hydrogen peroxide solutions and the effects of H 2 O 2 on Insulin peptide
36	Arzoo	IIT Bombay	Role of Hatree-Fock exchange in Proton Transfer
37	Sonali Mahadev Jadhav	IISER, Pune	Mechanistic study of the working of hexa-meric AAA+ Transporter GTPase McrB motor
38	Amol Tagad	IIT bombay	The selectivity of RAS; Mg2+, GTP and aspartic acid (119D) on the binding site
39	Soumak Ghosh	IACS Kolkata	Crucial role of explicit solvation in computational modelling of chemical reactions: Mechanism of Cu(I) transfer between thiolate-based chelators in water
40	Pragnya Samal	CSIR- NCL Pune	Modelling of adsorption properties for Zn-FAU, CALF 20 and MOF-74 towards enhanced CO2 separation from H2
41	Ritwika Dey	IIT Kharagpur	Interaction and dynamics of a glycosylated enzyme
42	Anjali Negi	IIT Kanpur	Theoretical Study of Structure, Dynamics, and Vibrational Spectroscopy of Aqueous Acetic Acid
43	Shubham Kumar	IISc Bangalore	Boltzmann’s H-Function and H-Theorem: Insights into Nonequilibrium Relaxation

SDCBS23:Posters

Session - 2 (27/10/2023, 05:20PM-07:00PM)

Poster No.	Name	Affiliation	Poster Title
1	Hema Teherpuria	IIT Jodhpur	Salt Concentration Effects on Ion Aggregation in EC-LiTFSI Electrolytes
2	Ramsha Javed	IIT Kanpur	Bucket Sampling: A New Sampling Approach to Sample High Dimensional Free Energy Landscapes
3	Khusboo Dubey	BITS Pilani Goa	Structure and Properties of Pyrrolidinium-Amino acid-based ionic liquids: A Computational Study.
4	Parna Roy	IISc Bangalore	Modeling of single photon emission fidelity of nanocrystal quantum dots
5	Subhadip Sahoo	IIT Kharagpur	Exploring the Effects of an Ionic Liquid on Aβ Peptide in Its Monomeric and Aggregated states
6	Abhinav Gupta	IIT Kanpur	Study of the molecular mechanism of proteolysis reaction by SARS-CoV-2 main protease, M^pro, enzyme via multiple pathways using parallel bias temperature accelerated sliced sampling (PBTASS) approach: A QM/MM study
7	Nandeshwar	IIT Dhanbad	Probing potential inhibitors of Amylin: A computational study
8	Gourab Saha	IIT Kharagpur	Exploring the Conformational Properties of a β-barrel Protein and the Confined Environment in and around It
9	Smita Manjari Panda	IIT Dhanbad	An in-silico approach to finding a potent inhibitor against mutated BRCA1
10	Subhajit Dan	IIT Kanpur	Terahertz Sum Frequency Generation Spectroscopy of Air-Water Interface Using Polarizable Force Field
11	Raju Sarkar	IISER Kolkata	Hierarchical Hydration Dynamics in RNA Stabilize its Functional Tertiary Motifs
12	Deepak Kumar Mahanta	IIT Bhubaneswar	The Behaviour of Ionic Liquids and Their Mixture on Protein and Water Structure
13	Satyendra Rajput	IIT Delhi	Ethylene glycol energetically destabilizes aggregates of pseudoisocyanine dyestuffs at crowded concentrations
14	Suman Bhowmik	IIT Kanpur	Effect of H-bonding and Viscosity on Intersystem Crossing Dynamics of a Rigid Aromatic Carbonyl Compound: Potential Role of Vibration
15	Arun Chakrabortty	IIT Kharagpur	Computational Investigations of Poly(A)-Binding Protein Complexed with Poly(A) RNA
16	Subhadip Banerjee	NISER Bhubaneswar	Effect of Electronegative Atoms on π – π Stacking and Hydrogen Bonding Behavior in Simple Aromatic Molecules - An Ab Initio MD Study
17	Amal Vijay	IISER Pune	Effect of arginine enantiomers on RNA tetraloop folding: Evidence for hypothesis on RNA-based origin of homochirality
18	Divya Rai	IIT Kharagpur	Impact of dimerization on the structure and dynamics of human carbonic anhydrase IX: Insights from classical molecular dynamics simulations
19	Tushar Singh Verma	NCL Pune	Supported transition metal-based DAC as an efficient NRR catalysts: Potent combinations as identified through computational screening
20	Amrita Chakraborty	IISER Kolkata	Effects of Fuzzy Interactions on RNA-peptide Complex Formation in Immunodeficiency Viruses
21	Akhilesh Shyamdhar Jaiswar	IISER Kolkata	Thermodynamics of Magnesium Chelation in RNA

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Poster No.	**Name**	**Affiliation**	**Poster Title**
22	Mahabul Haque	NIT Meghalaya	HSA-mediated Synthesis of CdTe Quantum Dots: Anti-bacterial, Cell Cytotoxicity Studies and Biosensing Applications
23	S A M Shamimul Ahsan	ADM	Designing an intermolecular potential for accurate description of pore size distribution in 12-ring siliceous zeolites
24	Rumela Adhikary	IACS Kolkata	Mechanistic Details of Spontaneous Hierarchical Self-assembly of Helical Nanofibers and Role of Water in the Assembly
25	Tanmoy Khan	IIT Kanpur	Why do Proteins Remain Stable and Active in Deep Eutectic Solvents?
26	Kore Shivshankar Mallappa	CSIR- NCL Pune	Elucidation of pH-Induced Protein Structural Changes: A Combined 2D IR and Computational Approach
27	Anushree Sinha	IISER Kolkata	Nodding Dynamics of SARS-CoV-2 Prefusion Spike Head Varies with Variants of Concern: Elucidating by Developing Sym-SBM Coarse-grained
28	Abhilash Chandra	IIT Kanpur	Theoretical Vibrational Sum Frequency Generation Spectroscopy of Liquid-Vapour Interfaces of Aqueous Solutions of Monovalent and Divalent Metal Nitrates
29	Ritama Kar	IIT Kanpur	Modelling Chemical Reactions using Molecular Dynamics at the Fourth Rung of DFT Functionals
30	Sumitava Kundu	IACS Kolkata	Particle shape determines the orientational disorder of the entropic crystals
31	Archy Tripathi	Ruhr Univ., Germany	Simulating a Solid para-Hydrogen Matrix using Path Integrals
32	Kumari Kiran	IIT Madras	Ionic-liquid based Nano-Composite Film for Biomedical Applicationss
33	Rimjhim Moral	IIT Guwahati	A Comparative Study of the Stability and Behaviour of Cyclic Peptide Nanotubes in Different Lipid Bilayers using MD Simulation
34	Jaya Vasavi Pamidimukkala	IIT Madras	A comprehensive computational approach in predicting the viral epitopes by targeting the MHC-TCR complexation
35	Subhasmita Mahapatra	IIT Indore	Molecular Dynamics Simulations Reveal Phosphorylation-induced Conformational Dynamics of the Fibroblast Growth Factor Receptor 1 Kinase
36	Saumyak Mukherjee	Ruhr Univ., Germany	Molecular thermodynamics of protein condensate formation from all-atom MD simulations
37	Nikhil Gupt	IIT Kanpur	Floquet Quantum Thermal Transistor
38	Aritra Mitra	IIT Guwahati	Transition Path Theory Reveals the Mechanism of α-Amyloid Formation in hll-37_17-29 Peptides
39	Himanshu Kumar Vishwakarma	IIT Kanpur	Terahertz spectroscopic studies of aqueous MgCl2 and CaCl2 solutions from molecular simulations using polarizable models
40	Kunal Shewani	IISER Bhopal	Mechanistic insights into G-protein activation via phosphorylation mediated non-canonical pathways
41	Prashant K Pandey	IIT Kanpur	Molecular mechanism and kinetics of the process of evaporation at liquid-vapor interface of aqueous solutions
42	Shuvadip Ghosh	IIT Kanpur	Quantum Thermal Switch and Rectifier
43	Sameer Saurav	IIT Kanpur	Host-Guest Binding Free Energies from Temperature Accelerated Sliced Sampling Simulations
44	Shitanshu Bajpai	IIT Kanpur	Temperature Accelerated Sliced Sampling using OpenMM