Symposium on

Molecular Simulations of Complex Fluids and Interfaces

February 21 – 23, 2020

Indian Institute of Technology Kanpur

Presenter	Title of the Poster
Shubham Tiwari	Insight to the Mechanism of Nanoparticle Induced Suppression of Detergency: Theory and Simulations
Hrushikesh M. Gade	Water-mediated curvature change in graphene by single-walled carbon nanotube: A molecular dynamics study
Avula Venkata Siva Nikhil	Atomistic Modeling of Binary Ionic Liquid Mixtures
Prosun Halder	High Throughput Screening of Hypothetical Metal Organic Frameworks for Ethane-Ethylene Separation
Sonali Gore	Tuning the adsorption behaviour of the material at the molecular scale to get the desired macroscopic behaviour by using statistical mechanics and molecular simulations
Shakkira Erimban	Cold Adaptation of Cell Membrane of a Psychrotolerant Bacteria: Investigation using Molecular Dynamics Simulation
Vikas Dubey	Mechanism of Hydroxide Ion Transfer through Anion Exchange Membrane in Anion Exchange Membrane Fuel Cell: Investigation using Molecular Dynamics Simulation
Nirali Dhiren Desai	New age antimicrobial peptides: Revealing mode of

	actions of multifunctional AMPs using molecular dynamics study
Shivam Dueby	Role of Translational Jump-diffusion in the Breakdown of the Stokes-Einstein relation in Supercooled Water and its Binary Mixture with Glycerol
Omkar Singh	Characterization of biological water at interface of antimicrobial peptide in presence of salts solution
Arya Das	Molecular Dynamics Simulations on Interfacial Structure in Presence of Third Component
Projesh Kumar Roy	Microscopic structure and CO_2 adsorption properties of 6FDA/BPDA-DAM polymeric membrane
Gauri Tekbahadur Thapa	Molecular dynamics simulation of anti-HIV protein SAMHD1
Bharti	Melting in two-dimensional Gay-Berne liquid crystals
Manjinder Singh	A comparative study of Tackifying Monomers to develop Bio-Based Pressure-Sensitive Adhesive: A Computational Approach
Ravi Kumar Reddy A	Uncovering the molecular mechanism of solvent induced polymorphism in crystal nucleation from solution
Jyoti Kuntail	Understanding the Adsorption Mechanism of Arsenous acid on Magnetite (311) Surface through Molecular Dynamics simulations
Rajneesh Kashyap	Oil Detachment from Rock Surface using Nanoparticles, Surfactant and low salinity brine: A Molecular Dynamic Study
Shivanand Kumar Veesam	Molecular Modelling of Phase Equilibrium of Gas Hydrates
Jagroop Kaur	Temperature Dependent Interaction of Soft Repulsive Wall with the Thermotropic Liquid Crystals
Krishna Jaiswal	A Functional Force Field Model for Water based on Gaussian Charges

Sanchari Bhattacharjee	Effect of Alkyl chain on The Wetting Behaviour of Aqueous Ionic Liquids: A Molecular Dynamics Study
Shubhandra Tripathi	A temperature accelerated Sliced Sampling study of Drug Binding/Unbinding
Sagar Dinkar Kamble	Investigation of Cholesterol influence in fluid phase and gel phase lipid bilayers by Coarse-grained Molecular Dynamic simulation
Showkat Mir	Electronic properties of high CO2 capture ability of two-dimensional metal nitrides (XN; X=Al, Ga, In): a computational study
Amrita Goswami	Formulation and Implementation of General Topological Network Criteria for Exploring the Structures of Confined Ice
Nandlal Pingua	Topological Identification Criteria, Stability and Relevance of Pentagonal Nanochannel in Amorphous Ice
Anil Mangla	A Thermodynamic Perspective of order-disorder transition of Ni_3Fe
Debabrata Pramanik	Understanding complex biomolecular systems using enhanced sampling techniques