



RECENT ADVANCES IN COMPUTATIONAL CHEMISTRY

SOLID STATE AND STRUCTURAL CHEMISTRY UNIT
INDIAN INSTITUTE OF SCIENCE, BENGALURU

MEETING DETAILS

Monday, 4th December 2017	
09:15-09:30	<i>Inauguration/Welcome</i>
Session 1	
09:30-10:00	<i>Stochastic Dynamics in Condensed Matter: Neutron Scattering and Molecular Dynamics Simulation Studies</i> R. Mukhopadhyay , BARC, Mumbai
10:00-10:30	<i>Understanding Protein-DNA Interactions from Molecular Simulations</i> Sanjoy Bandyopadhyay , IIT-Kharagpur, Kharagpur
10:30-11:00	Break
11:00-11:30	<i>Paracetamol aggregation on biocompatible polymers – Role of Topology and Interactions</i> Manju Sharma , University of Hyderabad, Hyderabad
11:30-12:00	<i>Fast Ion Transport in Solids: Insights from Recent Molecular Dynamics Studies</i> P. Padma Kumar , IIT-Guwahati, Guwahati
Lunch (at Main Guest House): 12:15 to 14:00 hours	
Session 2	
14:00-14:30	<i>Diffusion of Guest Moving Through Window Under Encapsulation</i> Pradip Kr. Ghorai , IISER-Kolkata, Kolkata
14:30-15:00	<i>Lattice Dynamics and Anomalous Thermal Properties</i> S. L. Chaplot , BARC, Mumbai
15:00-15:30	Break
15:30-16:00	<i>Sub-Arrhenius Diffusion in Binary Colloidal System</i> A. V. Anil Kumar , NISER, Bhubaneswar
16:00-16:30	<i>Active Particle Condensation and Confinement by Nonreciprocal and Time-delayed Interactions</i> Ahmed Sayeed , University of Pune, Pune
16:30-17:00	High Tea
17:00-18:30	Felicitation Function