



SYMPOSIUM on Structure and Dynamics

Under the auspices of UKIERI (UK-India Education and Research Initiative)



Day 1: December 10 (Monday), Raman Hall

09:45 -10:45	Registration and High Tea
10:45 -10:50	Welcome Remarks – Prof. BSM Rao, IISER Pune
10:50 -11:40	Keynote Address: Prof. K. N. Ganesh, Director, IISER Pune
Session 1: Chairperson – Prof. K. N. Ganesh, IISER Pune	
11:45 -12:15	Fast dynamics in biomolecules: overturning some well established ideas <i>Prof. Klaas Wynne, University of Glasgow</i>
12:15 -12:45	Mechanisms of substrate recognition by nucleic acid binding enzymes <i>Dr. Mrinalini Puranik, IISER Pune</i>
12:45 – 13:15	(π^*,σ^*) -Triplet Excited States – From Cyclic Disulfides to Atmospheric Chemistry <i>Dr. Goetz Bucher, University of Glasgow</i>
Lunch (13:15 – 14:30 hrs)	
Session 2: Chairperson – Prof. B. S. M. Rao, IISER PUNE	
14:30 -15:00	Local structure studies of functional metal oxides <i>Dr. Serena A. Corr, University of Glasgow</i>
15:00 -15:30	Polymer Vesicles: Design Principle, Encapsulation Capabilities and Delivering of Anticancer Drugs <i>Dr. M. Jayakannan, IISER PUNE</i>
15:45 – 18:00	Poster Session and Tea (Mendeleev Block)

Day 2: December 11 (Tuesday), Raman Hall

Session 1: Chairperson – Prof. Klaas Wynne, University of Glasgow	
9:30 - 10:00	The spectroscopy of the big: Using sculpted EM fields to probe mesoscale chirality <i>Dr. Malcolm Kadodwala, University of Glasgow</i>
10:00 - 10:30	Molecular level study of non-covalent interactions: Gas phase laser spectroscopy and quantum chemistry calculations <i>Dr. Alope Das, IISER PUNE</i>
10:30 - 11:00	Modulation of excited State photophysics of biologically important guests by the macrocyclic hosts <i>Dr. Partha Hazra, IISER PUNE</i>
11:00 -11.20	Tea
Young Investigator Session : Chairperson - Dr. Mrinalini Puranik, IISER PUNE	
11:20 - 11:40	Biomolecular structure from Raman optical activity (ROA) spectroscopy <i>Dr. Chris Syme, University of Glasgow</i>
11:40 - 12.00	Non-linear chiroptical spectroscopy of chiral plasmonic nanomaterials <i>Mr. Calum Jack, University of Glasgow</i>
12:00 - 12:20	Thermodynamic stability, reactivity and spectra of methane gas hydrates from electronic structure calculations <i>Ms K. R. Ramya IISER PUNE</i>
12:20 - 12:40	Mimicking trimeric interactions in the aromatic side chains of the proteins: A gas phase study of indole...(pyrrole) ₂ heterotrimer <i>Mr. Sumit Kumar, IISER PUNE</i>
12:40 – 13:00	In-vitro probing of protein-DNA interaction through fluorescence switch of an eminent anticancer drug: Ellipticine <i>Mr. Abhigyan Sengupta, IISER PUNE</i>
Lunch (13:00 – 14:30 hrs)	
Session 2: Chairperson - Dr. Malcolm Kodadwala, GLASGOW UNIVERSITY	
14:30 - 15.00	Insights into enzymatic catalysis using computational chemistry: From docking to coupled-cluster methods <i>Dr. Hans Senn, University of Glasgow</i>
15:00 - 15:30	A computer simulation study of structure and dynamics in Polymer Electrolyte Fuel Cell Membranes <i>Dr. Arun Venkatnathan, IISER PUNE</i>
15:30 – 16:00	On-Surface Assembly of 2D Ionic Metal-Organic Layers <i>Dr. Nirmalya Ballav, IISER PUNE</i>
16:00	Tea

Day 3: December 12 (Wednesday), Raman Hall

Session 1: Chairperson- Dr. M. Jayakannan, IISER PUNE	
09:30 -10:00	Structural dynamism and functional studies of coordination polymers <i>Dr. Sujit Kumar Ghosh, IISER PUNE</i>
10:00 – 10:30	Ionic Motion and Chemical Reactions within Crystalline Lattices <i>Dr. Eddie Cussen, University of Strathclyde</i>
10:30 - 11:00	Entropy Balance in the Intercalation Process of an Anti-Cancer Drug Daunomycin <i>Dr. Arnab Mukherjee, IISER PUNE</i>
11:00 – 11:30	Tea
Session 2: Chairperson - Dr. Hans Senn, University of Glasgow	
11:30 – 12:00	Computational and Experimental Studies of Peptide Self-Assembly <i>Dr. Tell Tuttle, University of Strathclyde</i>
12:00 – 12:30	Perturbation with THz Light <i>Dr. Pankaj Mandal, IISER PUNE</i>
12:30 – 13:00	Nanowire Photonics: Plasmonic and Organic <i>Dr. G. V. Pavan Kumar, IISER Pune</i>
Lunch (13:00– 14:30 hrs)	
14:30 – 16:00	Concluding Session: Discussion on Collaborative Programmes and Planning for the meeting at Glasgow in summer 2013
16:00	Tea