1 Day Symposium on

MOLECULAR AND MESOSCALE SIMULATIONS: APPLICATIONS IN ENGINEERING SCIENCES

May 9, 2009, Venue : Faculty Hall
Indian Institute of Science, Bangalore 560 012

Session/Time	**Speaker**	**Title of the Talk**
8.30 am – 9.15 am	**REGISTRATON**	
9.15 am.	**Welcome Address: Prof. Prabhu R Nott, Indian Institute of Science, Bangalore**	
SESSION I	**DENSITY FUNCTIONAL METHODS**	
Session Chair	**Prof. Shobhana Narasimhan, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore**	
9.30 am - 9.55 am	Raj Ganesh, Indian Institute of Technology, Kanpur	Ask Not What You Can Do For The (Density Functional) Theory, But What The Theory Can Do For You
9.55 am - 10.20am	Kunj Tandon, Shell R&D, Bangalore	Modeling Surface Chemical Reactions in Catalysts
10.20 am - 10.45 am	S. Balasubramanian, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore	Computer Simulations of Room Temperature Ionic Liquids
10.45 am - 11.15 am	**TEA BREAK**	
SESSION II	**BIOLOGICAL SYSTEMS: MEMBRANES/DNA**	
Session Chair	**Prof. K.L. Sebastian, Indian Institute of Science, Bangalore**	
11.15 am – 11.40 am	Satyavani Vemparala, Institute of Mathematical Sciences, Chennai.	Ion Conduction and Drug Interactions in a Potassium Channel
11.40 am – 12.05 am	Prabal Maiti, Indian Institute of Science, Bangalore	Elasticity at Nanoscale: DNA Under Tension
12.05 am – 12.30 pm	P.B. Sunil Kumar, Indian Institute of Technology, Madras	Shear Induced Ordering in Branched Living Polymer Solutions
12.30 pm - 2.00 pm	**LUNCH - IISc GUEST HOUSE LAWNS**	
SESSION III	**MOLECULAR SIMULATIONS – II**	
Session Chair	**Prof. T.A. Abinandanan, Indian Institute of Science, Bangalore**	
2.00 pm - 2.25 pm	Sudeep Punnathanam, Indian Institute of Science, Bangalore	Activated Instability During Homogeneous Bubble Nucleation and Growth
2.25 pm - 2.50 pm	Pankaj Apte, Indian Institute of Technology, Kanpur	Direct Computation of Anisotropy of Crystal-Melt Interfacial Energy of Silicon by Simulation
2.50 pm - 3.15 pm	Jhumpa Adhikari, Indian Institute of Technology, Bombay	Prediction of Thermodynamic and Structural Properties of InGaAs Using Molecular Simulations
3.15 pm – 3.40 pm	Manisha Vekaria, Accelrys Software Inc., Cambridge.	Modeling Methods for Understanding Surface Science, Catalytic Processes and

		Corrosion Mechanisms
3.40 pm – 4.15 pm	**TEA BREAK**	
SESSION IV	**MESOSCALE AND CONTINUUM SIMULATIONS**	
Session Chair	**Prof. Sriram Ramaswamy, Indian Institute of Science, Bangalore**	
4.15 pm – 4.40 pm	P. Sunthar, Indian Institute of Technology, Bombay	Excluded Volume Cross-over Function of the Intrinsic Viscosity of a Dilute Solution of Polymers.
4.40 pm - 5.05 pm	Srinivas Mohan, Fluent, Pune	Discrete Particle Models for Dense Fluid-Particulate Flows
5.05 pm - 5.30 pm	Anugrah Singh, Indian Institute of Technology, Guwahati	CFD Simulation of Shear Induced Particle Migration