TCS10: DETAILED PROGRAM

DAY-1: *Dec. 9, Thursday*

09:00-09:30		Inauguration
9:30-10:00		**Tea**
Session 1		
Chair: S. K. Ghosh		
10:00-10:45	L1	Screening, Structure and Simulation of Coulomb Systems: The Long and Short of It ***John. D. Weeks***
10:45-11:30	L2	Binary Mixtures and Biology ***B. Bagchi***
11:30-11:50		**Tea**
Session 2		
Chair: S. Kumar		
11:50-12:20	L3	Chemical Reactivity Dynamics within a Quantum Fluid Density Functional Framework ***Pratim Chattaraj***
12:20-12:40	L4	Growth and stabilization of non-native ultrathin semiconducting films and transformation to native structure via depolarized surfaces ***Raj Ganesh S.Pala***
12:40-13:00	L5	Computational studies on Homogeneous Catalysis ***Anoop Ayyappan***
13:00-14:00		**Lunch**

DAY-1: *Dec. 9, Thursday (Cont.)*

Session 3		
14:00-16:00	P01 - P72	**Poster Session 1 + Tea**
16:00-16:45	L6	Playing with the buckyball ***N. Sathyamurthy***
16:45-17:30	L7	Ab initio-based potentials and dynamics within the Born-Oppenheimer approximation and beyond ***A. J. C. Varandas***
17:30-17:50	L8	Dynamical Insights into Heterogeneous Catalysis: Methane Dissociation on Metal Surfaces ***Ashwani K. Tiwari***
17:50-18:10	L9	Insights into the ligand discrimination, and switching mechanisms of SAM-III riboswitch via molecular dynamics simulations ***Deva Priyakumar***
18:10-18:30	**Tea**	
Session 5		
Chair: S. Kumar & S. Mahapatra		
18:30-19:30	Prof. N. Sathyamurthy's 60th Birthday Felicitation	
20:00-21:30	**Dinner**	

DAY-2: *Dec. 10, Friday*

Session 6		
Chair: Rama Kant		
09:00-09:45	L10	A design for a normal hydrogen electrode for density functional theory based molecular dynamics ***Michiel Sprik***
09:45-10:30	L11	Walking in the Brownian Storm ***M. S. Gopinathan***
10:30-11:00	**Tea**	
Session 7		
Chair: Parbati Biswas		
11:00-11:30	L12	Some New Approaches to Photon-Molecule Dynamics ***M K Mishra***
11:30-12:00	L13	Some Applications of Computational Chemistry ***E. D. Jemmis***
12:00-12:20	L14	Towards ab initio design of solar fuels ***Vardha Srinivasan***
12:20-12:40	L15	Structure and dynamics of water at the nanoscopic hydrophobic confinement ***Niharendu Choudhury***
12:40-13:00	L16	Striped Pattern Formation on Gold Nanoparticle Surfaces ***Pradip Kr. Ghorai***
13:00-14:00	**Lunch**	

DAY-2: *Dec. 10, Friday (Cont.)*

Session 8		
Chair: Sanjoy Bandyopadhyay		
14:00-14:45	L17	Hydrogen Molecule and Hydrogen Atom Under Strong Magnetic Fields ***B. M. Deb***
14:45-15:05	L18	Range-Separated Hybrid Density Functional Theory (RSH-DFT): A novel scheme to model weak interactions ***Prasenjit Seal***
15:05-15-25	L19	Anisotropic scattering patterns in semi-dilute polymer solutions under steady shear flow ***Prasanth Jose***
15:25-16:00	**Tea**	
Session 9		
Chair: Harjinder Singh		
16:00-16:30	L20	Molecular Tailoring: an Art of the Possible for *Ab Initio* Treatment of Large Molecules and Molecular Clusters ***Sridhar Gadre***
16:30-17:00	L21	Quantum diffusion in presence of Fermionic noise ***Deb Shankar Ray***
17:00-17:30	L22	The Klauder Phenomenon: Perturbative and Variational Implications ***Kamal Bhattacharyya***
17:30-17:50	L23	Molecular spin filter: A new paradigm of spintronics ***Swapan Chakrabarty***
17:50-18:10	L24	Low-lying Excitations of Poly-Fused Thiophene within Pariser-Parr-Pople Model: A Density Matrix Renormalization Group Study ***Mousumi Das***
18:10-18:30	**Tea**	
18:30-19:30	**Cultural Program**	
20:00-21:30	**Symposium Dinner**	

DAY-3: *Dec. 11, Saturday*

Session 10		
Chair: Srabani Taraphder		
9:00-9:45	L25	The dynamics of loop formation in a semiflexible polymer ***K. L. Sebastian***
9:45-10:30	L26	Computational Chemistry For Some Real Chem/Bio Problems: Reaction Mechanism of Explosives, Personalized Drug Design, Membrane Proteins and Protein-DNA Interactions ***Dongqing Wei***
10:30-11:00	**Tea**	
Session 11		
Chair: P. Venuvanalingam		
11:00-11:30	L27	Response function analysis of excited-state energy functionals ***M. Harbola***
11:30-12:00	L28	Human HIV-1 gp120 envelope glycoprotein interactions with receptor CD4: a molecular dynamics study ***Prabal Maiti***
12:00-12:20	L29	Solvent-Induced Dynamical Transition in Proteins ***Rajesh K. Murarka***
12:20-12:40	L30	Structure of Large Molecules in Solution: A multiscale modeling strategy ***Chandra N. Patra***
12:40-13:00	L31	Microscopic basis of heterogeneous enzyme catalysis ***Gautam Gangopadhyay***
13:00-14:00	**Lunch**	

DAY-3: *Dec. 11, Saturday (Cont.)*

Session 12		
14:00-16:00	P73-P144	**Poster Session 2 + Tea**
Session 13		
Chair: V. Subramanian		
16:00-16:30	L32	Effective Floquet Hamiltonians for dipolar and quadrupolar coupled N-spin systems in solid-state NMR under Magic Angle Spinning ***Mangala Sunder Krishnan***
16:30-17:00	L33	Structure and Properties of Impurity-doped Gold Clusters ***Tapan Ghanty***
17:00-17:20	L34	Study of Ion Binding of theHybrid Cyclic peptide Nanotubes ***P. Kolandaivel***
17:20-17:40	L35	Molecular Dynamics and Quantum Chemical Studies on Incremental Solvation of Glycine ***R. Kanakaraju***
17:40-18:00	L36	Explicitly time-dependent electron dynamics and its control ***R. Padmanaban***
18:00-18:20	L37	Theoretical Studies of Electronic Excitation Energy Transfer involving some Nanomaterials ***R. S. Swathi***
20:00-21:30	**Dinner**	

DAY-3: *Dec. 12, Sunday*

Session 14		
Chair: Narahari Sastry		
09:00-09:30	L38	Properties of excited states using highly accurate coupled-cluster methods ***Sourav Pal***
09:30-09:50	L39	Insights from helical propensity, cation-π and π-π interactions on the structure and function of peptides and proteins. ***Madhavi Sastri***
09:50-10:10	L40	Extracting the folding motif from functional β-trefoil proteins ***Sachi Gosavi***
10:10-10:30	L41	Differing Water Dynamics in the Grooves of DNA ***Subrata Pal***
10:30-11:00	**Tea**	
Session 15		
Chair: Ranjit Biswas		
11:00-11:30	L42	Single-file diffusion of subdiffusive particles ***Tusar Bandyopadhyay***
11:30-11:50	L43	Control of electron localization in molecules using attosecond pulse train and many-cycle IR pulse ***Kamal P. Singh***
11:50-12:10	L44	The intriguing chemistry of ammonia-borane dehydrogenation ***Ankan Paul***
12:10-12:30	L45	Effective Hamiltonians in Molecular spectroscopy ***Aniruddha Chakraborty***
12:30-12:50	L46	Coupled cluster Method for molecular properties ***Nayana Vaval***
12:50-13:00	**Concluding Remarks**	
13:00-14:00	**Lunch**	