A DISCUSSION MEETING ON "RECENT ADVANCES IN MOLECULAR SIMULATIONS"

List of Poster titles for 8th February 2018 (3:15 PM – 4:45 PM)

SL. NO.	TITLE	NAME OF THE STUDENT
P1	Phosphorylation Induces a Unique Conformation in Rap-Raf Complex by Allosteric Modulation of Switch Loop Dynamics	Devanand T
P2	Osmolyte Effects on the Growth of Amyloid Fibrils	N M Aswathy
P3	Modelling and Molecular Dynamics Study on LiM2IV(PO4)3 Where M= Zr, Hf, Sn, Ti	Krishnanjan Pramanik
P4	Interfacial Water Dynamics on Graphene Oxide Surface	M. Rajasekaran
P5	Tuning of singlet -triplet fission in tetracene through donor/acceptor substitution	Anusooya Pati
P6	Strategies to Extract the Conductance for Circuits Embedded within a Terpyridine Based Molecular Breadboard	Ravinder Kumar
P7	High Thermoelectric Performance in n-doped Silicon-Based Chalcogenide Si2Te3	Rinkle Juneja
P8	Towards Development of Generic Inhibitors Against Proteases of Picornaviruses via Simulation Based Studies	Ruchika Bhat
P9	Ferroelectricity, Antiferroelectricity, and Ultrathin 2D Electron/Hole Gas in Multifunctional Monolayer Mxene	Avanish Mishra
P10	Collective excitations in Water-Ethanol binary mixture: Composition dependent far-infra red spectrum, low frequency vibrational density of states, dielectric relaxation and dipolar solvation dynamics	Milan K. Hazra
P11	Microscopic Understanding of the Conformational Features of a Protein-DNA Complex	Sandip Mondal
P12	Hofmeister Effects on Protein Folding	Hiranmay Maity
P13	Phase Segregation in Two Temperature Lennard-Jones Type Systems: Molecular Dynamics Simulation	Siva Chari
P14	Markov State Model for Single-Molecule Force Spectroscopy	Susmita Ghosh
P15	Effects of Commensurability on a Monatomic Lennard-Jones Fluid Confined Between Structured Mica Walls - A Molecular Dynamics Study	V. Vadhana
P16	Slow-down of Water Dynamics at Narrow Carbon Nanotube-Water Interfaces	Srinivasa Rao Varanasi
P17	Temperature effects on the attractive force between two hydrophobic walls in water	Tuhin Samanta
P18	Molecular Dynamics Simulations Reveal the Role of Membrane Cholestrol During Pore Forming Pathway of Cytolysin A	Amit Behera
P19	Origin of Multiple Time Scales in Protein Hydration Layer Solvation Dynamics: Role of Protein Conformational Fluctuations	Sayantan Mondal
P20	TBA	Bharti Singh
P21	TBA	Shivani Gupta
P22	TBA	Manisha Jadon

A DISCUSSION MEETING ON "RECENT ADVANCES IN MOLECULAR SIMULATIONS"

List of Poster titles for 9th February 2018 (3:30 PM – 4:45 PM)

P1	Modelling Molecular Magnets with Large Exchange and Large on-site Anisotropy	Sumit Haldar
P2	Stabilization of Insulin Hexamer Assembly by Ten Confined Water Molecules	Saumyak Mukherjee
P3	PAMAM Dendrimer-Graphene Composites: Interesting Analogies with Star Polymers	Mounika Gosika
P4	Sub-Arrhenius Diffusion in a Binary Colloidal System	Mahammad Mustakin
P5	Translocation of Bioactive Molecules Through Carbon Nanotubes Embedded in Lipid Membrane	Anil Kumar Sahoo
P6	Tunable Two-Dimensional Interfacial Coupling in Molecular Heterostructures	Vivek K Yadav
P7	Interfacial Free Energy Calculations for Binary Hard Sphere Mixtures	Praveen Kumar Bommineni
P8	Influence of Dipole Moment and Pi Stacking on Energy of Thiophenation : A Gaussian Approach	Rabi Narayan Patra
P9	Contrasting Co-Solvent Effects on the Growth of Fibrils by Intrinsically Disordered Peptides and Globular Proteins	Balaka Mondal
P10	A Robust Model to Predict Thermodynamic Properties of Gas-Hydrates	Shivanand Kumar Veesam
P11	Calculation of Surface Tension at Solid-Liquid Interfaces	Ravi Kumar Reddy A
P12	Effect of ethanol on the stability of insulin dimers	Puja Banerjee
P13	How the Structure of Sodium Dodecyl Sulfate Micelles in Deep Eutectic Solvent Compare with that in Water	Aditya Gupta
P14	Complete Inhibition of Pt Site Poisoning and Efficient Carbon Monoxide Oxidation Induced by Vanadium and Cobalt	Rafia Ahmad
P15	Exact Wave Packet Dynamics of Singlet Fission in Unsubstituted and Substituted Polyene Chains Within Long-Range Interacting Models	Suryoday Prodhan
P16	Anomalous Diffusion of Hexane Isomers in Faujasite	Angela Mary Thomas
P17	Behavior of Reline Deep Eutectic Solvent in Confinement: A Molecular Dynamics Investigation	Supreet Kaur
P18	Charge transport in Nucleic Acids	Abhishek Aggarwal
P19	C2N/WS2 Van der Waals Type-II Heterostructure as a Promising Water Splitting	Ritesh Kumar
P20	TBA	Pavan Krishna Kanchi
P21	TBA	Surya Sekhar Manna
P22	TBA	S Shyam