

3rd North-West Meeting on Spectroscopy, Structure and Dynamics (SSD-2019)

Department of Chemistry
Indian Institute of Technology Roorkee

<p>5th April 2019 (Friday) (3:00-3:15 PM) Kulgeet Welcome & Overview of the Meeting: C. N. Ramachandran (<i>Convener SSD-2019</i>) Introduction of the Department: K. R. Justin Thomas (<i>Head, Department of Chemistry</i>) Address to the participants: Ajit K. Chaturvedi (<i>Director, IIT Roorkee</i>)</p>	
<p>Tea (3:15-3:30 PM)</p>	
<p>Outreach Lecture (3:30-3:55 PM) Ashwani Kumar Tiwari (IISER Kolkota) <i>Quantum dynamics on time-dependent and time-independent potential energy surfaces of certain molecules</i></p>	
4:00-4:25 PM	<p>V. Ramanathan (IIT-BHU) <i>Cu as a substrate for surface enhanced Raman Spectroscopy</i></p>
4:30-4:55 PM	<p>Saugata Hazra (IIT Roorkee) <i>Resounding OM using omics: Novel interdisciplinary approach to combat against antibiotic resistance</i></p>
5:00-5:15 PM	<p>Naveen Kumar (IISER Mohali) <i>Barrier localization of wave packet densities</i></p>
5:15-5:30 PM	<p>Renu Bala (IIT Roorkee) <i>Ab initio calculations of spectroscopic constants and properties of MgLi⁺ and CaLi⁺</i></p>
5:30-5:45 PM	<p>Ankita Joshi (IIT Roorkee) <i>Opto-electronic properties of cycloparaphenylene-carbon nanotube based molecular machines</i></p>
<p>Tea & Poster Presentations (5:45-6:45 PM)</p>	
<p>6th April 2019 (Saturday)</p>	
9:00-9:25AM	<p>Shamik Chakraborty (BITS Pilani) <i>Let's have isolation</i></p>
9:30-9:55AM	<p>Ananya Debnath (IIT Jodhpur) <i>Dynamics of chlorophyll aggregation in lipid membranes using coarse grained molecular dynamics simulations</i></p>
10:00-10:25AM	<p>Ashok Garai (LNMIIT Jaipur) <i>DNA nano-mechanics: Theory and simulation</i></p>
10:30-10:55AM	<p>Hemant Kumar Kashyap (IIT Delhi) <i>Theoretical understanding of capillary evaporation of ionic liquids in nanoscale solvophobic confinement</i></p>
<p>Tea (11:00-11:15 AM)</p>	
11:15-11:40AM	<p>Atul Kumar (IIT Jodhpur) <i>Analyzing correlations in two and three-particle states</i></p>
11:45-12:10 PM	<p>Manikandan Paranjothy (IIT Jodhpur) <i>Competing radical and molecular dissociation pathways of halons</i></p>
12:15-12:30 PM	<p>Subhasish Mallik (MNIT Jaipur) <i>Role of post-ccsd(t) corrections on the strongly correlated CH₃O+O₂ system</i></p>
12:30-12:45 PM	<p>Bhawna Chaubey (IIT Jodhpur) <i>Structural Transition of aqueous Melittin in presence of Trifluoroethanol: A NMR relaxometry approach</i></p>

Lunch (1:00-3:00 PM)	
3:00-3:25 PM	Samanwita Pal (IIT Jodhpur) <i>Estimation of proton transfer (PT) rate of uracil derivative in an entrapped environment: A three site vs. two site exchange model</i>
3:30- 3:55PM	Krishna Mohan Poluri (IIT Roorkee) <i>Characterizing the structure-function relationship of bacteriophage endolysin using biophysical methods</i>
Tea and Poster Presentation (4:00 – 5:00 PM)	
Visit to Haridwar and Dinner (5:00 - 10:00 PM)	
7th April 2019 (Sunday)	
9:00-9:25AM	Anirudha Chakraborty (IIT Mandi) <i>Multistate problems in quantum and statistical mechanics-analytically solvable models</i>
9:30-9:55AM	Prashant Uday Manohar (BITS Pilani) <i>Cholesky representation of Fock-Space MRCC constraints in variational linear response for analytical dipole moment and polarizability</i>
10:00-10:25AM	Pallavi Debnath (IIT Roorkee) <i>Dynamics in polymer liquids</i>
10:30-10:55AM	Pradeep Kumar (MNIT Jaipur) <i>Effect of confinement on the dissociation of carboxylic acids</i>
Tea Break (11:00 AM- 11:15 AM)	
11:20-11:45AM	Ravindra Pandey (IIT Roorkee) <i>Probing the density of states at buried interfaces with even order spectroscopy</i>
11:50AM- 12:10 PM	Vinit (IIT Roorkee) <i>Spin spin coupling and spin polarization in fullerene derivatives</i>
12:15-12:30 PM	Concluding Remarks