



## Research Scholar's Day 2022

Department of Chemistry, IIT Kanpur Date: April 09<sup>th</sup>, 2022; Venue: L-20 Lecture-Hall

09:30 AM	Inauguration: Prof. Jitendra K. Bera, Head, Department of Chemistry				
	Session I (09:40-11:00) Chair: Dr. Arnab Ghosh				
09:40–10:00	Ms. Apurva Panjla: Anionic diketopiperazine as a potent osteoinductive molecule				
10:00–10:20	Mr. Shovon Chatterjee: Single step green synthesis of methylammonium lead bromide nanocrystals				
10:20–10:40	Ms. Sabeeha Parveen: Coinage metal complexes of dimesitylboron containing 2-(diphenylphosphino)-1-methylimidazole				
10:40–11:00	Mr. Manmohan Shukla: Sc(OTf)3-catalyzed synthesis of symmetrical dithioacetals and bisarylmethanes				
	Tea Break (11:00-11:30)				
	Session II (11:30-12:50) Chair: <i>Dr. Dharmaraja Allimuthu</i>				
11:30–11:50	Ms. Nidhi Sorout: Effects of BN nanoparticles & selected osmolytes on the secondary structure of A $\beta$ -peptide in aqueous medium				
11:50–12:10	Mr. Arindom Bhattacherya: Hydrogenation of CO <sub>2</sub> and Urea Derivatives to Methanol Using Proton Responsive Ru(II)-NHC Pincer Catalyst				
12:10–12:30	Ms. Usha Yadav: Luminescent lanthanide sensors for the detection of chemical biological warfare agents				
12:30–12:50	Mr. Rohit K. Maurya: Femtosecond laser-induced thermal spectroscopy for investigating molecular interactions in liquids				
	Lunch Break (13:00-15:00)  Session III (15:00-16:20) Chair: <i>Dr. Apparao Draksharapu</i>				
15:00–15:20	Ms. Khyati Shukla: Enantioselective synthesis of tetrahydrofuran spirooxindoles via domino oxa-Michael/Michael addition reactions using a bifunctional squaramide catalyst				
15:20–15:40	Mr. Ashok Kumar: The curious case of tetrachloropalladate – structure, packing and order-disorder transitions				
15:40–16:00	Ms. Kasturi Ganguli: Cyclometalated Ru(II) complexes towards functionalization of alcohols and ketones with methanol				
16:00–16:20	$\emph{Mr. Ankush Gupta}$ : Total Syntheses of 6-Amino-2,6-dideoxy- $\alpha$ -Kdo and related compounds				
	Session IV (16:20-17:00) Chair: <i>Dr. Nagma Parveen</i>				
16:20–16:50	Prof. Srihari Keshavamurthy: The challenge of staying curious in research and teaching				
16:50–17:00	Vote of Thanks: President, Chemical Society				
	Session V (17:00-18:30) Chairs: Drs. Devendra Mani, Parthasarathi Subramanian, Prakash C. Mondal, and Vishal G. Rao				
17.00-18.30	Poster Session and High Tea (17:00-18:30)				
	RSD activities ends at 18:30 hours				

## Poster Presentations

Poster Number	Presenter	Title of the Poster		
P-01	Abhijit Manna	Asymmetric synthesis of spiro 3,3'-cyclopropyl oxindoles via vinylogous Michael initiated ring closure reaction		
P-02	Abhishek Kumar Yadav	Di-cationic Nitrogen-rich Triazole and Tetrazole-Based Energetic Salts: Synthesis and Detonation Performance		
P-03	Anirban Sau	Chemoselective Reductive Methylation of $\alpha,\beta\textsc{-Unsaturated}$ Ketones using Methanol		
P-04	Anubhav Nath	A Protic Mn(I) Complex Based on Naphthyridine-N-oxide Scaffold: Protonation/Deprotonation Studies and Catalytic Applications for Alkylation of Ketones		
P-05	Arghya Sen	Conversion of Colloidal 2D Ruddlesden-Popper Iodide Based Perovskite Nanoplates into 3D Nanocrystal: An Insight into Ligand-Nanocrystal Surface Binding		
P-06	Ashwini Kumar	Role of Iron Chelators and Their Transmetalative Approach for the Design and Engineering of Potential Therapeutics		
P-07	Ayushi Awasthi	Spectroscopically deciphering the formation of a fleeting Ni(III) bisphenoxyl diradical complex		
P-08	Chhavi Khajuria	Brønsted acid-catalyzed reaction between C-alkynyl imine precursor and thiol: Access to highly enantioenriched propargyl amides		
P-09	Deepannita Samanta	An approach to decipher the stability of bis-Fe(IV) MauG		
P-10	Dharmendra Kumar Yadav	Hydrogen peroxide - inducible PROTAC for the degradation of epidermal growth factor receptor in cancer		
P-11	Diksha Srivastava	Two-dimensional molecular materials for electronic applications		
P-12	Hariom Birla	Effect of functional group on the switching efficiency of azobenzene derivatives on graphite		
P-13	Himanshu Sonker	Design, synthesis, and therapeutic application of 2- Hydroxy-1- naphthaldehyde Schiff base compounds, utilizing bioconjugation strategies		
P-14	Ishani Borthakur	A Selective and Sustainable Synthesis of Secondary and Tertiary Amines by Reductive Alkylation of Azides/ Nitroarenes		
P-15	Kajal Chaudhary	Utilizing ferroptosis phenomenon to influence tumor progression and facilitate anti-biofilm cancer mitigation therapies		
P-16	Maheswar Reddy G.	Solvatochromic effect on photophysical properties of Imidazolin-5-one containing $\pi$ -conjugated push-pull system		
P-17	Monika Ahlawat	Bimetallic Nanocomposites as an Engineered Plasmonic Catalyst		
P-18	Nidhi Garg	Dehydrogenative Methanol Activation and its application as Transfer Hydrogenating reagent under homogeneous catalysis		
P-19	Nidhi Gupta	Study of intermixing effect in Ge/Si(001) growth using kinetic Monte Carlo simulations		

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P-20	Nikhil Gupt	Statistical generalization of regenerative quantum		
		Stirling cycle		
P-21	Parasar Kumar	Unexpected Synthesis of Oxadiazole Analogues:		
		Characterization and Energetic Properties		
P-22	Priya	Anisotropic quantum drude oscillator model for van der		
		Waals corrections over a cheap density functional		
P-23	Ramsha Javed	Bucket Sampling: A New Approach to Compute High		
		Dimensional Free Energy Landscapes		
P-24	Ranjeev Kumar	All-organic molecular electrochromic devices for fast, thr		
	Parashar	states colour-switching with high coloration efficiency		
D 25	Ritama Kar	Molecular Dynamics at the Fourth Rung of DFT Jacob's		
P-25		Ladder Made Two Orders of Magnitude Faster		
P-26	Saikat Pal	$\alpha$ -alkylation of Nitriles with Primary and Secondary		
		Alcohols by Hemilabile Mn(I) Complex		
	Sayantani Banerjee	Stabilization of Axial Phenoxide Radical in a Ni(II)-Fe(III)		
P-27		Heterobimetallic Porphyrin Dimer: An Experimental and		
,		DFT Investigation		
	Shiwangi Maurya	Genome analysis and growth kinetics of a non-marine		
P-28		halotolerant methylotrophic bacterium <i>Paracoccus sp.</i>		
		strain DMF		
P-29	Sikha Gupta	Synthesis and spectroscopic characterization of a Mn(III)		
		O-Ce(IV) intermediate		
	Sona Tiwari	Modulating reactivity of isotoic anhydrides between lysin		
P-30		and cysteine using chemical handles		
		Iron-catalyzed Wacker-type Oxidation of Olefins Under		
P-31	Sourav Pal	Ambient Conditions		
	Syed Jehanger Shah Tanmoy Khan	Chlorin π-Cation Radical Dimer: A Synthetic Model of		
P-32		Bacteriochlorophyll Special Pair Antenna		
		Is a sugar polyol alter the spatial and dynamic		
P-33		heterogeneity in a non-ionic deep eutectic solvent? Clue		
		form translational, rotational and solvation dynamics		
P-34	Vaishali Thakkur	-		
		Inhibition Mechanism of Class D $\beta$ -Lactamases by Avibactam		
P-35	Change Death	Intramolecular Proton Transfer in Pyridoxal 5'-Phosphate		
	Shreya Rastogi	Schiff Bases at the Active Site of Ornithine Decarboxylase		
		A QM/MM Metadynamics Study		
P-36	Prashant K Pandey	Molecular mechanism and kinetics of the process of		
		evaporation at liquid-vapor interface of aqueous solution		

End of the	Posters List	
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