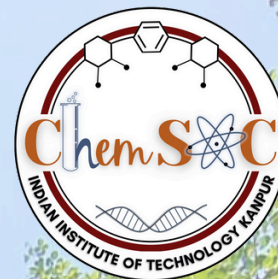


# RESEARCH SCHOLAR DAY 2025



Department of Chemistry

IIT kanpur



May 08, 2025



Outreach Auditorium

|                          |                    |
|--------------------------|--------------------|
| <b>Inaugural address</b> | <b>9:30 - 9:45</b> |
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| <b>Session 1</b> | <b>9:45 - 10:45</b> |
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**Session chair: Ritama Kar**

| <b>Time</b>   | <b>Speaker</b> | <b>Title of the talk</b>                                                                                                                                                  |
|---------------|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 9:45 – 10:00  | Nitin Sharma   | Concise Enantioselective Total Syntheses of Rearranged ent-Trachylobane Diterpenoids (-)-Wallichanol A and B                                                              |
| 10:00 – 10:15 | Riya Gupta     | Water Clusters in Superfluid Helium Nanodroplets                                                                                                                          |
| 10:15 – 10:30 | Sourav Bag     | Ligand-Controlled Cobalt-Catalyzed Hydroboration of (Poly)carbonates for the Synthesis of Value-Added Chemicals                                                           |
| 10:30 – 10:45 | Zahid Ahmed    | Asymmetric Aza-Michael/Michael/Mannich Domino Reaction of 2-Aminochalcones and 5-Alkenyl-Thiazolones: Access to Enantioenriched 1,4-Sulfur-Bridged Piperidinone Skeletons |

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| <b>Tea-break</b> | <b>10:45 - 11:00</b> |
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| <b>Poster Session 1: P1 – P15</b> | <b>11:00 - 11:45</b> |
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| <b>Session 2</b> | <b>12:00 - 12:45</b> |
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**Session chair: Deepannita Samanta**

| <b>Time</b>   | <b>Speaker</b>   | <b>Title of the talk</b>                                                                          |
|---------------|------------------|---------------------------------------------------------------------------------------------------|
| 12:00 – 12:15 | Adarsha Mandal   | Pincer-(NHC)Mn(I) Complex-Catalyzed Activation of Alcohols Molecules Toward Sustainable Synthesis |
| 12:15 – 12:30 | Farha Naaz       | Data-mining and high-throughput approaches to predict novel perovskite materials                  |
| 12:30 – 12:45 | Saurabh K Rajput | Functional N-Centered Persistent Organic Radicals                                                 |

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| <b>Lunch Break</b> | <b>12:45 - 14:00</b> |
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**Session 3****14:00 - 14:45****Session chair: Tanmoy Khan**

| <b>Time</b>   | <b>Speaker</b>    | <b>Title of the talk</b>                                                                           |
|---------------|-------------------|----------------------------------------------------------------------------------------------------|
| 14:00 – 14:15 | Neha Clare Minj   | Repurposed Cu-Scrap as An Anode for The Electrooxidation of Small Molecules                        |
| 14:15 – 14:30 | Soumyadip Saha    | Kinetic Monte Carlo (KMC) Simulations of Gallium Nitride (GaN) Growth on m-plane (1-100)           |
| 14:30 – 14:45 | Patralekha Sarkar | Pivotal Role of Interfacial Binding in Ultrafast Hole Transfer from Halide Perovskite Nanocrystals |

**Session 4****15:00 - 15:45****Session chair: Suraj Kashyap**

| <b>Time</b>   | <b>Speaker</b> | <b>Title of the talk</b>                                                                                                                                                 |
|---------------|----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 15:00 – 15:15 | Shantanu Sen   | Seeing is believing: Proposing A Self-Investigated Insulin Quality Monitoring Method                                                                                     |
| 15:15 – 15:30 | Anjali Negi    | Structure and Intermolecular Interactions at Liquid-Vapor Interfaces of Aqueous Osmolyte Solutions through Theoretical Vibrational Sum-Frequency Generation Spectroscopy |
| 15:30 – 15:45 | Vikrant Vini   | Non-Covalent Stapling of Oligopeptides by Tuning Aromatic Amino Acid Residues                                                                                            |

**High Tea****16:00 - 17:00****Poster Session 2: P16 – P29****16:15 - 17:00**

**Colloquium**

**17:00 - 18:00**

**Session Chair: Priya**

**Speaker**

**Title of talk**

Prof. Srihari Keshavamurthy    Dreaming of mode-specific chemistry – inside a “box”?

**Vote of thanks**

**18:00 - 18:15**

• Poster session 1

| No. | Speaker            | Title of poster                                                                                                                                                                   |
|-----|--------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| P1  | Rhitwika Chowdhury | Ambient CO <sub>2</sub> Cycloaddition to Challenging Epoxides via Hydroxypyridine functionalized Zinc-Imidazolium Catalysts: A Pathway to Renewable Cyclic Carbonates             |
| P2  | Ayusie Goyal       | Prussian blue analogue heterointerface on a pre-oxidized copper foam surface for enhanced anodic oxidation performance                                                            |
| P3  | Goutam Panigrahi   | Differential binding interactions of physiological phosphates on macrocyclic luminescent Eu(III) probes via simultaneous VET/PeT process                                          |
| P4  | Sayari Dewan       | Self-Assembling Imidazolium Nanoaggregates Trigger a Unique Dynamin-Dependent Cell Death via Cytoplasmic Vacuolization and Mitochondrial Dysfunction in Human Lung Adenocarcinoma |
| P5  | Divya Mahapatra    | Co(II)-Catalyzed Additive-Free Transfer Hydrogenation of N-Heteroarenes at Room Temperature                                                                                       |
| P6  | Uttej Sai Krishna  | Polycyclic and Spiro-Dihydroquinones Induce Lipid Peroxidation to Prevent Cancer Cell Proliferation                                                                               |
| P7  | Chirantan Singha   | Biomimetic Synthesis of Cucurbalsaminone A                                                                                                                                        |
| P8  | Amit Kumar Sharma  | Dynamic Kinetic Resolution in Ring-opening Cyclization of Aziridines: Enantioselective Route to Benzodiazepines                                                                   |
| P9  | Subhajit Dan       | Study of Sum Frequency Generation Spectroscopy of Water in the Terahertz region using Polarizable Force Field                                                                     |
| P10 | Pankaj Kumar       | Enhancing the Efficacy of Photocatalytic Reduction Reaction with 'Strongly Coupled' Nanoscale Plexciton Hybrid                                                                    |
| P11 | Shuvadip Ghosh     | Inverse Current in Coupled Transport                                                                                                                                              |
| P12 | Vijay Bahadur      | Nitrogen Doping through Precursor Selection for Improving the Charge Transport in Transferable Semi-Conducting 2D-imine Covalent Organic Framework                                |
| P13 | Sandip Paul        | Femtosecond Laser Induced Thermal Lens Spectroscopy for Sensing Liquid-Air Interface                                                                                              |
| P14 | Priya              | A Green's function formalism for kinetic energy density functional in Orbital-free DFT                                                                                            |
| P15 | Pooja Rani         | 1-Methyl Imidazole Clusters in Superfluid Helium Nanodroplets                                                                                                                     |

• Poster Session 2

| No. | Speaker            | Title of poster                                                                                                                                                     |
|-----|--------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| P16 | Abhik Ghoshal      | Counterions Drive Memory Functionality in Two-terminal Viologen-based Molecular Junctions                                                                           |
| P17 | Tamal Kanti Biswas | Visible Light-Mediated Acceptor-less Dehydrogenative Coupling for the Synthesis of Quinolines and Naphthyridines Using a Perimidine-Based Iron(II) Catalyst         |
| P18 | Deepannita Samanta | Unusually Stable Synthetic Diheme bis-Fe(IV)oxo: An Intermediate in Diheme Enzymes MauG and BthA                                                                    |
| P19 | Sneha Mittal       | Developing High-Performance OER Electrode via an Eccentric Corrosion of NiFeCo Substrate                                                                            |
| P20 | Sumedha Gupta      | Multifunctional surfactants derived from amino acids: the effect of pH and temperature on their interactions with bovine serum albumin                              |
| P21 | Vatsalya Gupta     | Benzyl thioether-based trans-thioetherification as a dynamic covalent motif for designing covalent adaptable networks                                               |
| P22 | Anshika Sinha      | Haloalkane-driven dichotomous reactivity of aryl radicals as halogen and hydrogen atom transfer agents: photocatalytic olefin and alkyne functionalization cascades |
| P23 | Sameer Saurav      | Kinetics of Barrier Crossing Events from Temperature Accelerated Sliced Sampling Simulations                                                                        |
| P24 | Riya Rathore       | Unravelling the properties of perovskites through ab initio approaches                                                                                              |
| P25 | Sandipan Maitra    | From Atom to Island: Simulating Silicene Growth on Ag(III) with DFT and kMC                                                                                         |
| P26 | Shivani Gupta      | Enhanced Photocatalysis via Perovskite-Molecular Synergy and Surface Engineering                                                                                    |
| P27 | Bhupendra Singh    | Protein Associated Water is Responsible for Maintaining the Stability of Eye Crystallin                                                                             |
| P28 | Aanchal Grover     | Second-Order Saddle Points and Concerted Reaction Mechanism: Insights from Entangled Trajectory Molecular Dynamics                                                  |
| P29 | Geetanjali Negi    | SARS-CoV-2 Evolved Variants Bind to Sialylated Gangliosides and Inhibited by Tetravalent Sialo-Glycocluster                                                         |