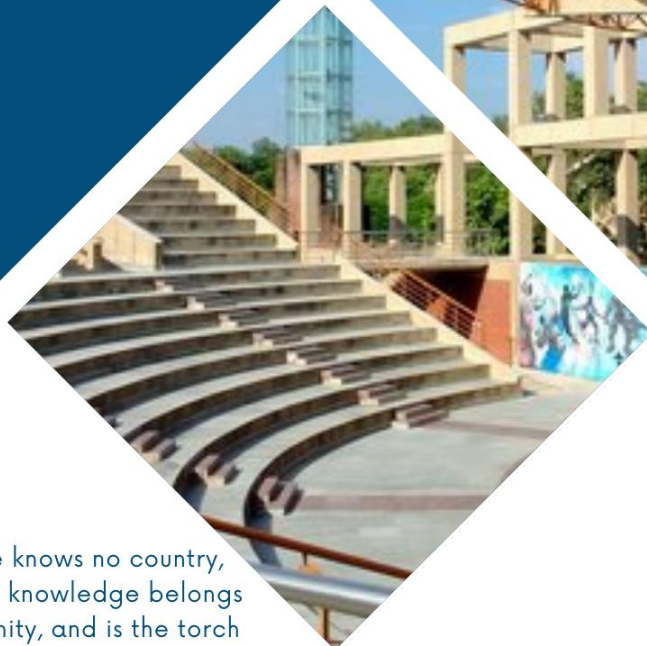


JOIN US  
**IN SHAPING THE  
FUTURE OF SCIENCE  
TOGETHER!**



"Science knows no country,  
because knowledge belongs  
to humanity, and is the torch  
which illuminates the world."  
- Louis Pasteur

# RESEARCH SCHOLAR DAY 2024

 **APRIL 19TH, 2024**

 **OUTREACH AUDITORIUM**

Discover our top pick of topics and speakers.  
Something for everyone. Something for you.

Action Potentials,  
Neuromodulation, and  
Wireless Neuroengineering  
Communication

**-PROF. S. VERMA**

Asking Ligands to  
Lend a hand

**-PROF. J. K. BERA**

**DISCOVER STUDENT  
EXCELLENCE: ORAL &  
POSTER PRESENTATIONS  
AWAIT!**



## Research Scholars Day-2024: Program Schedule

Day: 19 April 2024, Friday, 09:10 hrs

Forenoon sessions moderator: Mrs. Sai Kumari Vechalapu		
Time, hrs	Event	
09:10	Welcome and Inaugural address	
Session-1: Chair: Dr. Venkata Suresh Mothika		
	Speaker	Title
9:25	Prof Sandeep Verma	Potentials, Neuromodulation, and Wireless Neuroengineering Communication
Session-2: Chair: Ms. Jesila		
10:10	Mr. Vatsalya Gupta	Dynamic Covalent Polymeric Networks derived from PET waste and sustainable sources
10:30	Mr. Subhadip Mondal	Chemistry with Quantum Light: Cavity Mediated Modulation of Vibrational Energy Flow Pathways
10:50	Ms. Rhitwika Chowdhury	Hydroxypyridine Functionalized Tris-chelate Co(III)-NHC Complex: A Novel Catalyst for Cycloaddition of CO <sub>2</sub> to Epoxides
11.10-12.00	Poster Session-I Coupled with Tea Break	
Session-3: Chair: Ms. Pragya Katiyar		
12:00	Ms. Deepti Singh	Catechol 2,3-dioxygenase isoenzymes from Diaphorabacter sp. DS2 demonstrate different substrate preferences
12:20	Ms. Alka Karn	Development of Porous Organic Polymers (POPs) and Their Applications as Heterogeneous Organocatalyst

12:40 Mr Manoj Kumar Dispirocyclic Orthoester via an Acetal Oxo-Carbenium Ion: Total Syntheses of Aculeatins A, B, D, and 6-epi-D

13.00 to  
14.40

**Lunch Break**

**Afternoon Sessions Moderator: Mr. Abhishek Yadav**

**Session-4: Chair: Ms. Pragya Arora**

14:40 Mr. Abir Das Sustainable Strategies in Cobalt Catalysed Enantioselective C-H Bond Functionalization

15:00 Mr. Nitin Shukla Luminescent Lanthanide Coordination Polymer as a Dual-Mode Sensor for Nitro Explosive and Solid-State Sebaceous Fingerprint Detection

15:20 Ms. Priya A new formalism to calculate the kinetic energy density in OF-DFT using Green's function

**Session-5: Chair: Mrs. Sona Tiwari**

15:40 Ms. Diksha Srivastava Large Area Film of Highly Crystalline, Cleavable, and Transferable Semi-Conducting 2D-imine Covalent Organic Framework on Dielectric Glass Substrate

16:00 Ms. Deepannita Samanta Diheme Enzyme MauG: Nature's Sniper for Long-range Electron Transfer and Cooperative Catalysis

16:20 Mr. Sumit Kumar Gupta Probing of molecular interaction in carboxylic acids through thermal lensing

16-40 to  
17.30

**Poster Session-II and High-Tea**

**Session-6: Chair: Dr. Anantharaj Sengeni**

17:30 **Prof. Jiten K. Bera** Asking Ligands to Lend a hand

18.15

**Thanking Remarks**

**Poster Presentations: Session I: 11:10 to 12:00 hrs**

<b>Name</b>	<b>Poster number</b>	<b>Title</b>
Sathyapriya	<b>01</b>	Diazepam-based covalent modifiers of GPX4 induce ferroptosis in liver cancer cells
Anindya Sarkar	<b>02</b>	Hg-Hg-Hg interactions stabilize unusual Trinuclear Double Sandwich Structure of Mercury(II) porphyrins.
Divya	<b>03</b>	High Valent Pseudopeptide Copper Complex with Dangling Hypochlorite
Anubhav Nath	<b>04</b>	Efficient Dehydrogenation of Formic Acid under Base-free Conditions with the aid of a Novel Co(III) Complex Supported by a Highly Nucleophilic N-Heterocyclic carbene (NHC) Ligand
Samir Das	<b>05</b>	Floquet Quantum Transistor: Full Counting Statistics
Parasar Kumar	<b>06</b>	Zwitterionic fused pyrazolo-triazole based high performing energetic materials
Archana Yadav	<b>07</b>	Copper(I) and Ruthenium(II) complexes of Bioinspired Ligands of Hard and Soft Donors: Xanthates and Dithioformates from Metal-Borohydrides
Monika Ahlawat	<b>08</b>	Role of Interfacial Interactions in Harvesting Light from CsPbBr <sub>3</sub> Nanocrystals Through Oxidation of Primary Amines
Kavita Choudhary	<b>09</b>	Silver-Catalyzed Asymmetric Double Desymmetrization via Vinylogous Michael Addition of Prochiral $\alpha,\alpha$ -Dicyanoalkenes to Cyclopentendiones
Ranjeev Kumar Parashar	<b>10</b>	'All-organic' Electrochromic Devices For Fast Color-switching With High Coloration Efficiency
Ankita Jaiswal	<b>11</b>	SERS Based bio screening Platform for Selective Detection of $\beta$ -Amyloid peptide
Shitanshu Bajpai	<b>12</b>	Temperature Accelerated Sliced Sampling in OpenMM
Kirti	<b>13</b>	Excited State Pd-Catalyzed Reductive Alkylation of C=N Bond of Quinoxalin-2(1H)-ones /Oxazepine
Sunny Gautam	<b>14</b>	Electronic Properties of Pd doped surface confined metal organic network of Ferrocene derivatives.
Sadhan Dey	<b>15</b>	Reusable Cobalt-Catalyzed Selective Transfer Hydrogenation of Azoarenes and Nitroarenes
Ayushi Chaudhary	<b>16</b>	Cellular Accumulation and Endoplasmic Reticulum Localized Cyclometalated Iridium (III) Complexes as efficient Ferroptosis inducers
Kedar Yadav	<b>17</b>	Computational Structure-Property Correlations in Solid State Materials
Abhijit Saha	<b>18</b>	Tuning the Electronics of Bis-(tridentate)Ru(II)-complexes for ROS Generation: Modification to the Ligand Skeleton with Varying Aromaticity Beyond the Classical Extended pi-Conjugation
Vineet kumar	<b>19</b>	Manganese-Catalyzed Stereoselective Insertion of Allenyl Carbonates/Alcohols: Towards Z-Selective Allylation of Indole Derivatives
Nitin Sharma	<b>20</b>	Enantioselective Total Synthesis of Atisane Diterpenoids: (+)-Sapinsigins H, (+)-Agallochaol C, and (+)-16 $\alpha$ , 17-dihydroxyatisan-3-one
Deepika Sahi	<b>21</b>	<i>Ab initio</i> Molecular Dynamics and Machine Learning Study of Aqueous NaOH Solution
Susanta Kumar Behera	<b>22</b>	Organocatalytic Surfactants for Direct Asymmetric Aldol Reactions in Aqueous Media

Subhadip Pramanik	23	Control of Spin Coupling Through Imidazolate Bridge in Diiron(III) Porphyrin Dimer
Kiran	24	Probing the spectroscopic feature of Formal Nickel(IV) bis-amido pseudo-peptide complex

**Poster Presentations: Session II: 16:40 to 17:30 hrs**

Name	Poster number	Title
Sourav Bag	01	Ligand-Driven Manganese Catalyzed Hydroboration Reactions with Broad Substrate Scope
Shreyasi Banik	02	Facile fabrication of 1,3,4-oxadiazole and fused pyrazole based advanced high energy density material
Siddharth Singh	03	Synthesizing alkene via light induced dehydrohalogenation and halide exchange reaction in CsPbX <sub>3</sub> NCs.
Nidhi Saini	04	Organocatalytic Asymmetric Cascade Michael-acyl Transfer Reaction between 2-Fluoro-1,3-diketones and 2-Hydroxynitrostyrenes
Manajit Mandal	05	Induced Chirality in inorganic nanomaterials for enhanced optical and magneto-electrochemical phenomena
Rakhi Bormon	06	Anti-proliferative, -migratory and -clonogenic effects of long-lasting nitric oxide release in HepG2 cells
Vaishali Thakkur	07	A transition state guided methyl substituted beta-lactam framework approach for beta-lactam antibiotics and beta-lactamase inhibitors
Parashuram Sharma	08	Photoinduced LMCT alkylation and alphaaminoalkylation of coumarins
Nidhi Rawat	09	Photo induced trans-cis switching of azobenzene derivative on graphite surface.
Srabani Nandi	10	Regioselective Ring Opening of Epoxide with Alcohols: A Selective Route to $\alpha$ -Alkylated Ketones and $\beta$ -Alkylated Secondary Alcohols
Kajal Chaudhary	11	Ruthenium p-cymene derived metalloantibiotics with potent antimicrobial activity against resistant strains
Farha Naaz	12	Data mining-cum-first-principles theoretical approaches for perovskites
Soumen Paira	13	Mn(I) Cinchona catalyzed Asymmetric Hydrogenation of Ketones and Its Derivatives
Amar Uike	14	Ru(II)-Catalyzed Deoxygenative Formal [3 + 1 + 2] Benzannulation of Allyl Alcohols and Acetylenediester via C-H Activation and Selective Carbon-Carbon Triple Bond Cleavage
Akshay Kaushik	15	Structure and Dynamics of Aqueous Solutions of a Strong Acid using <i>Ab initio</i> Molecular Dynamics and Machine Learning Potentials
Abhishek Singh	16	A spectrophotometric trimethylamine monooxygenase assay
Arati Maurya	17	Exploring the Multifaceted Role of <i>N, N</i> -dimethylformamidase (DMFase): From Oligomeric Structures to Catalytic Mechanisms
Ashwini Kumari Shaw	18	Luminescent Lanthanide-Based Diagnostic Probes for Bioactive Anions

Geetanjali Negi	<b>19</b>	Disruption Mechanisms of Enveloped Viruses by Ionic and Nonionic Surfactants
Garvita Dhanwat	<b>20</b>	Calcium Mediated Protein Reconstitution Using Giant Plasma Membrane Vesicles as Fusogen
Sujan Singha	<b>21</b>	Investigations of hydrogen bonds formed by linear and antiparallel-(TH <sub>3</sub> CN) <sub>2</sub> (T = C, Si, Ge ) dimers
Deepak Singh	<b>22</b>	Role of AcrAB-TolC and its components in Influx-Efflux dynamics of QAC drugs in <i>Escherichia coli</i> revealed using SHG Spectroscopy
Sandip Paul	<b>23</b>	Comparative study of femto-second and CW optical trapping of nano-particle
Viral Rawat	<b>24</b>	Synthesis and decomposition evaluations of triazoles, a potential lysine/tyrosine modifiers

# **Students' Oral presentation Abstracts**