



Major Areas of Research/Up to 3 major sponsored projects

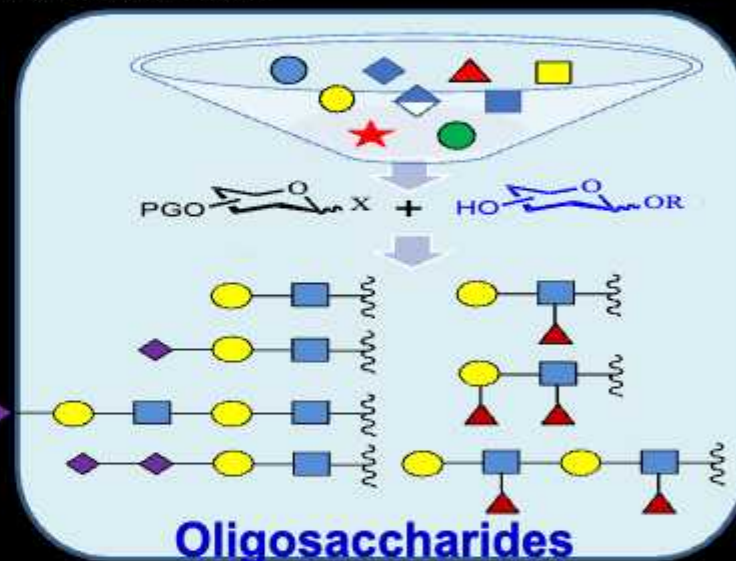
- 1) Development of synthetic strategy for carbohydrate based bioactive molecules
- 2) Development of Glyco-tools for potential drug delivery to the tumor cell
- 3) Electrochemical glycosylation: A green approach to access oligosaccharides

Major Research Facilities in the Group

- 1) 0°C to -80°C Low constant reaction bath with stirrer
- 2) Electrochemical Flow Reactor (will procure)
- 3) Automated flash column chromatography (will procure)

Technology/Product Developed/Up to 3 most significant Publications

- 1) A. Sau, R. Williams, C. Palo-Nieto, A. Franconetti, S. Medina, M. C. Galan. "Palladium-Catalysed Direct Stereoselective Synthesis of Deoxyglycosides from Glycals" *Angew. Chem. Int. Ed.*, **2017**, *56*, 3640-3644.
- 2) C. Palo-Nieto, A. Sau, M. C. Galan. "Gold (I) Catalysed Stereoselective Synthesis of Deoxyglycosides" *J. Am. Chem. Soc.* **2017**, *139*, 14041-14044.
- 3) A. Sau, K. Nagrajan, B. Patrahau, L. Lethuillier-Karl, R. Vergauwe, A. Thomas, J. Moran, C. Genet, T. W. Ebbesen "Modifying Woodward-Hoffmann Stereoselectivity under Vibrational Strong Coupling": *Angew. Chem. Int. Ed.*, **2021**, *60*, 5712-5717.



Arup Mahata

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Advanced Materials Laboratory, , Department of Chemistry

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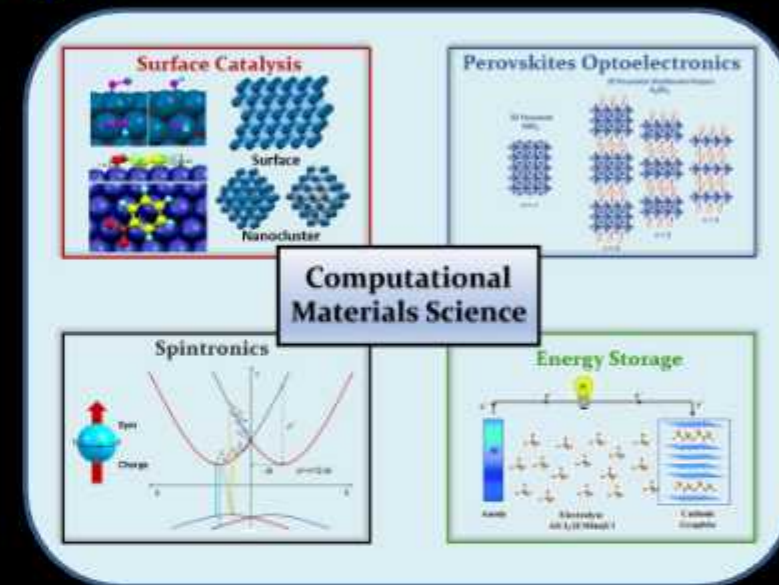
Computational Materials Science, First-Principles Calculations, Density Functional Theory, Perovskites Optoelectronics, Energy Storage Materials, Surface Catalysis (Electrochemical, Photoelectrochemical, Thermochemical), Molecular Catalysis, Spintronics

Major Research Facilities in the Group

Computational Chemistry Open Source DFT Software packages (Quantum Espresso, CP2K, ORCA, NWChem)

Technology/Product Developed/Up to 3 most significant Publications

1. A. H. Proppe, A. Johnston, S. Teale, **Arup Mahata**, R. Quintero-Bermudez, E. H. Jung, L. Grater, T. Cui, T. Filleter, C. Y. Kim, S. O. Kelley, F. De Angelis, E. H. Sargent, Multication perovskite 2D/3D interfaces form via progressive dimensional reduction, **Nat. Commun.** 2021, 12, 3472
2. **Arup Mahata**,* E. Mosconi, D. Meggiolaro, F. De Angelis, Modulating band alignment in mixed dimensionality 3D/2D perovskites by surface termination ligand engineering, **Chem. Mater.** 2020, 32, 105–113.
3. Y. Yang, C. Liu, **Arup Mahata**, M. Li, C. Roldan-Carmona, Y. Ding, Z. Arain, W. Xu, Y. Yang, P. A. Schouwink, A. Zuttel, F. De Angelis, S. Dai, M. K. Nazeeruddin, Universal approach toward high-efficiency two-dimensional perovskite solar cells via a vertical-rotation process, **Energy Environ. Sci.** 2020, 13, 3093–3101.



Ashutosh Kumar Mishra



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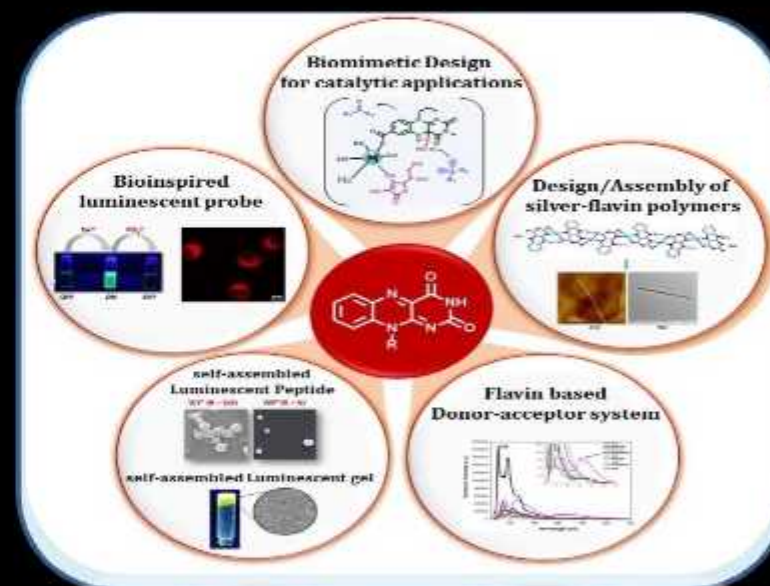
- ❖ Biomimetic synthetic design for catalytic transformations
- ❖ Bioinspired luminescent probe for bioimaging and sensing applications
- ❖ Design and functionalization of Metal-organic framework

Major Research Facilities in the Group

- ❖ Optical Microscope
- ❖ Fluorimeter
- ❖ High performance liquid chromatography (HPLC)

Technology/Product Developed/Up to 3 most significant Publications

- ❖ Design and synthesis of Flavin-Samarium complex as efficient photocatalyst for sulfoxidation reactions, Mouli, Katyal and Mishra Synlett, 2022, DOI: 10.1055/a-1928-3417
- ❖ Formation of the silver-flavin coordination polymers and their morphological studies. Mouli and Mishra, CrystEngComm, 2022, 24, 2221-2225
- ❖ Modulating catalytic activity of a modified flavin analogue via judiciously positioned metal ion toward aerobic sulfoxidation. Mouli and Mishra, RSC Adv., 2022, 12, 3990



Dr. Bhabani Shankar Mallik



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Indian Institute of Technology Hyderabad



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Major Areas of Research

Molecular Dynamics (Classical and DFT), AIML

Development of machine learning potential

Energy (Electrode and Electrolytes)

Catalysis (HER, OER, NRR and CO₂RR)

Energetic materials and ultrafast spectroscopy

Major Research Facilities in the Group

NSM-HPC facility at IIT Hyderabad

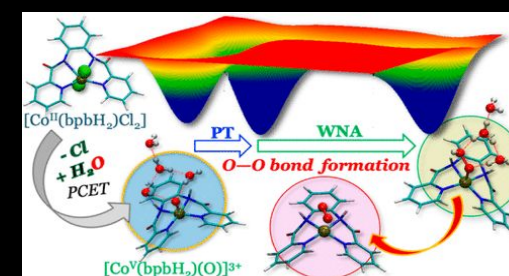
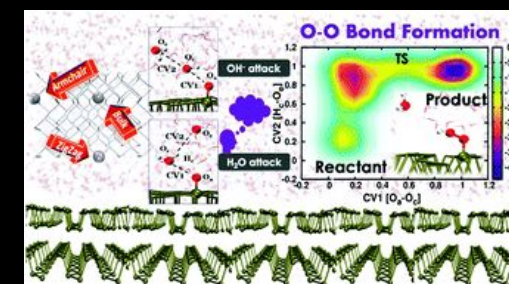
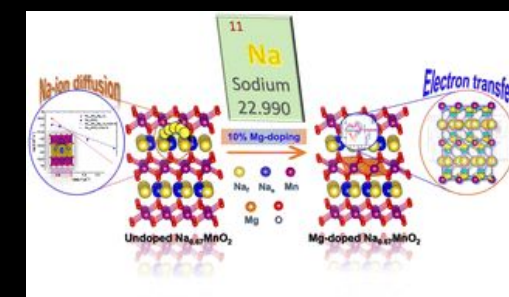
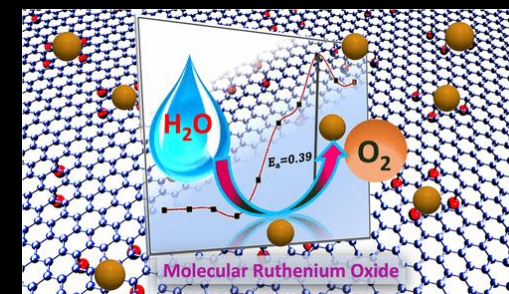
High performing servers

Most significant Publications

Adyasa Priyadarsini *et. al*, *J. Phys. Chem. C* **2023**, 127, 18350–18364

Aritri Biswas *et. al.*, *J. Phys. Chem. B* **2023**, 127, 1, 236–248

Dhileep N. Reddy *et. Al.*, *Phys. Chem. Chem. Phys.*, **2017**, 19, 10358-10370



C Malla Reddy

Professor , FlextalLab, Department of Chemistry



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Major Areas of Research/Up to 3 major sponsored projects

Core Research Grant by DST on “Exploration of Mechanically Flexible Organic Single Crystals in Flexible Opto-Electronic Devices” Amount: 1.02 Core (2021-2024; DST-SERB/CRG/004992)

Swarnajaynti Fellowship by DST, on “Designing Mechanical Behaviour of Functional Organic Crystals” Amount: INR ~ 2.49 crore (2016-2021; graded as Excellent).

Major Research Facilities in the Group

Nanoindentation Facility for measuring elastic modulus and hardness of small volumes of materials



Hot-stage microscopy attached with a high-speed camera for recording slow motion videos at different temperatures

Three most significant Publications

C.M. Reddy, *et. al. Science*, 2021, 373, 321-327

C.M. Reddy, *et. al. Nat Commun*, 2023, 14, 6589

C.M. Reddy, *et. al. Chem. Soc. Rev.* 2022, 49, 8878

RESEARCH

REPORT

Science

MATERIALS SCIENCE

Autonomous self-repair in piezoelectric molecular crystals

Surojit Bhunia^{1,2}, Shubham Chandel^{3†}, Sumanta Kumar Karan⁴, Somnath Dey⁵, Akash Tiwari³, Susobhan Das¹, Nishkarsh Kumar³, Rituparno Chowdhury¹, Saikat Mondal^{1,2}, Ishita Ghosh¹, Amit Mondal¹, Bhanu Bhushan Khatua⁴, Nirmalya Ghosh^{3*}, C. Malla Reddy^{1,2*}

Living tissue uses stress-accumulated electrical charge to close wounds. Self-repairing synthetic materials, which are typically soft and amorphous, usually require external stimuli, prolonged physical

Reddy *et al*, *Nature Chemistry*, 2015, 65–72

Self-healing cycle
FlexTal Lab, IIT Hyderabad
Prof. C. Malla Reddy

Debasish Koner



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Major Areas of Research

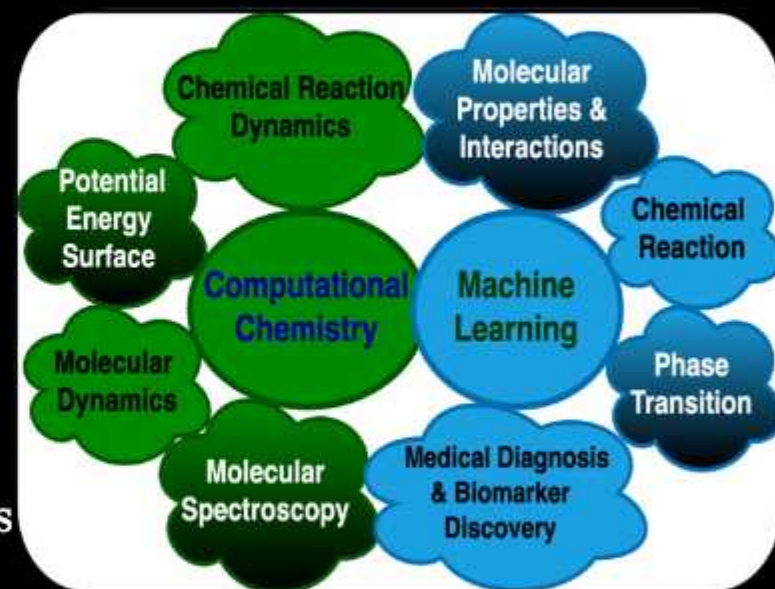
- Machine Learning in Chemistry
- Chemical Reaction Dynamics
- Molecular Spectroscopy
- AI Driven Medical Diagnosis and Biomarker Discovery
- Atmospheric and Astro-chemistry

Major Research Facilities in the Group

- Institute High Performance Computing (HPC)
- Computational Chemistry softwares
- AI and ML softwares

Up to 3 most significant Publications

- Koner, D. Quantum and quasiclassical dynamical simulations for the Ar_2H^+ on a new global analytical potential energy surface *J. Chem. Phys.* 154, 054303 (2021)
- Koner, D.; Meuwly, M. Permutationally Invariant, Reproducing Kernel-Based Potential Energy Surfaces for Polyatomic Molecules: From Formaldehyde to Acetone *J. Chem. Theory Comput.* 16, 5474-5484 (2020)
- Koner, D.; Unke, O. T.; Boe, K.; Bemish, R. J.; Meuwly, M. Exhaustive state-to-state cross sections for reactive molecular collisions from importance sampling simulation and a neural network representation. *J. Chem. Phys.* 150, 211101 (2019)





Melepurath Deepa

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Major Areas of Research: Applied Electrochemistry: Solution Processed Solar Cells, Batteries, Supercapacitors, Electrochromic Devices, Photoelectrochromic Devices, Photo-supercapacitors

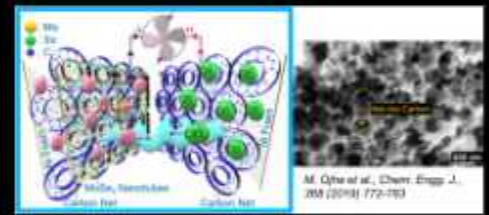
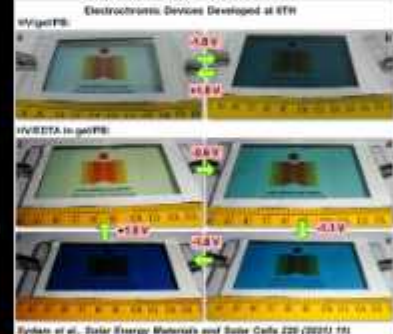
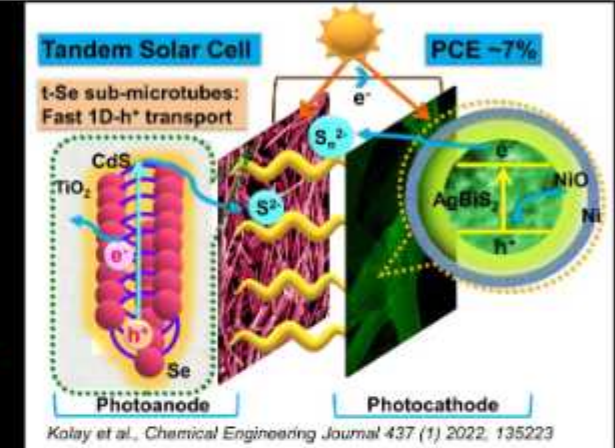
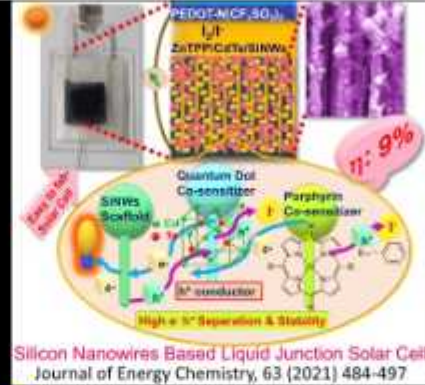
Major Research Facilities in the Group: Class

AAA Solar Simulator, IPCE Measurement facility, UV-Vis, Fluorescence spectrometers, Battery Testers, Electrochemical Workstations, Freeze Dryer, Microwave Reactor, Glove Boxes, Pouch cell supercapacitor fabrication facility, Furnaces, Ovens, Stirrers, Rotary Evaporator, Chiller etc

Technology/Product Developed:

- Developed pouch cell supercapacitor [at TRL: 4-5].
- Developed and demonstrated a prototype electrochromic device (~8 cm x 5 cm) with switching between blue and transparent states [at TRL-6].

Developed quasi-solid state low cost quantum dot solar cell with an efficiency of ~10%.



Faiz Ahmed Khan

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Major Areas of Research

- * Discovery of new methodologies and their evaluation for biological application.
- * Synthesis of natural and aesthetically pleasing unnatural products.
- * Chemical synthesis in ionic liquids and supported catalysts.

Selected Publications

Direct α -Benzylation of Methyl Enol Ethers with Activated Benzyl Alcohols: Its Rearrangement and Access to (\pm)-Tetrahydronyasol, Propterol A, and 1,3-Diarylpropane *J. Org. Chem.* **2019**, 84, 21, 14270–14280. (DOI: [10.1021/acs.joc.9b02064](https://doi.org/10.1021/acs.joc.9b02064))

Synthesis and antibacterial activities of marine natural product ianthelliformisamines and subereamine synthetic analogues *Bioorg. Med. Chem. Lett.* **39**, **2021**, 127883. DOI: [10.1016/j.bmcl.2021.127883](https://doi.org/10.1016/j.bmcl.2021.127883)

Solvent controlled synthesis of 2,3-diarylepoxo indenones and α -hydroxy diarylindanones and their evaluation as inhibitors of DNA alkylation repair *Org. Biomol. Chem.*, **2022**, 20, 5820–5835. DOI: [10.1039/D2OB00595F](https://doi.org/10.1039/D2OB00595F)

Boron Trifluoride Etherate-Controlled Reactions of Methyl Enol Ethers: Selective Synthesis of Dihydrofuro[3,2-c]chromenone and Furo[3,2-c]chromenone Derivatives *Synlett* **2022**, 33. DOI: [10.1055/a-1912-3884](https://doi.org/10.1055/a-1912-3884)

Major Research Facilities in the Group



IKA-ElectraSyn 2.0

Flash Chromatography Multivial Reactor



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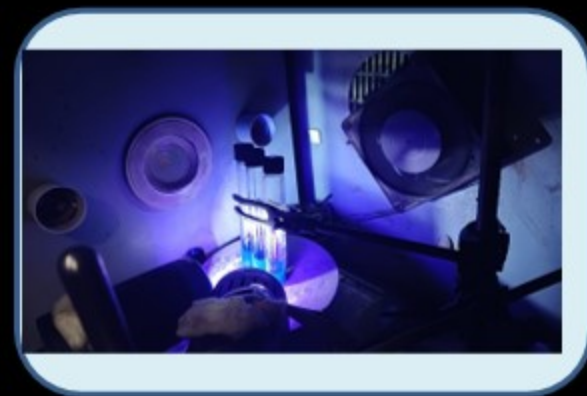
Major Areas of Research: Organic Synthesis

- 1) Transition-metal Catalysis
- 2) C-H Activation
- 3) Green Chemistry and Domino Cyclization
- 4) Development of New Methodology and Drug Diversity-Oriented Synthesis
- 5) Electrochemical Organic Synthesis
- 6) Photocatalysis

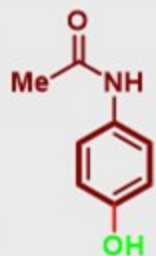


Major Research Facilities in the Group

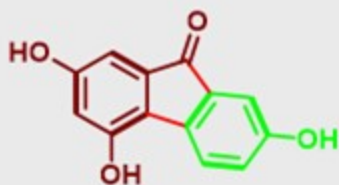
- 1) ElectraSyn 2.0
- 2) Microwave synthesizer
- 3) Photocatalysis set-up
- 4) Fume hood, Rotary evaporators, Magnetic Stirrers



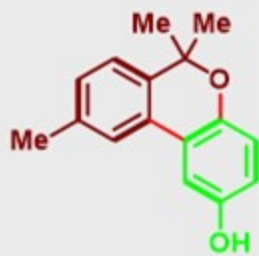
Technology/Product Developed



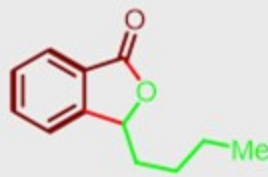
Paracetamol
(Drug)



4-O-Demethyl-nobilone
(Natural product)



Didehydroconicol
(Natural product)



"Butylphthalide (NBP)
(Anti-platelet drug)



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Jai Prakash

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Major Areas of Research

1. Metal chalcogenides
2. Thermoelectric materials
3. Superconducting materials
4. Small molecule crystallography

Major Research Facilities in the Group

1. Glove box
2. Programmable furnaces
3. Vacuum sealing line
4. Hydrothermal autoclaves

Publications

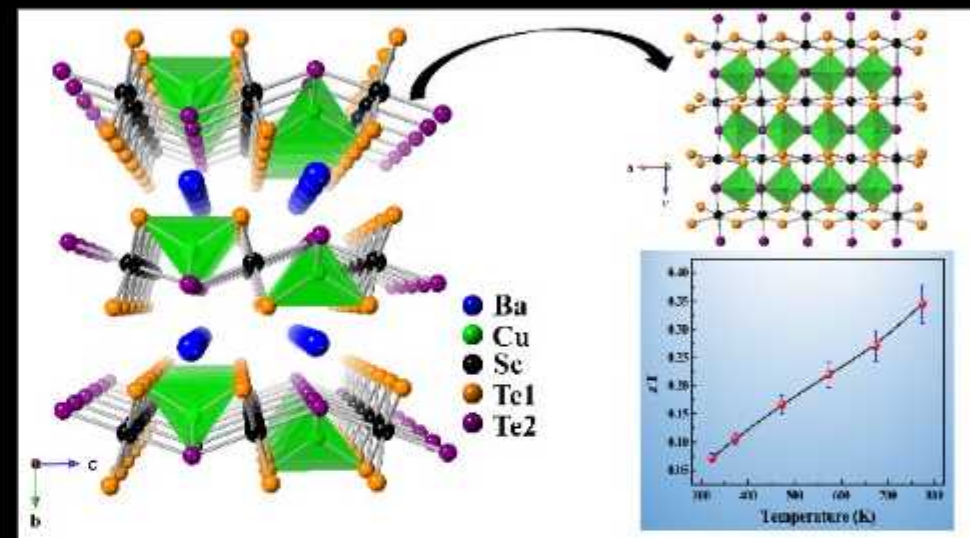
1. Subhendu Jana, Gopabandhu Panigrahi, Mohd Ishtiyak, S. Narayanswamy, Pinaki P. Bhattacharjee, Manish K. Niranjana, and **Jai Prakash**,

Germanium Antimony Bonding in $\text{Ba}_4\text{Ge}_2\text{Sb}_2\text{Te}_{10}$ with Low Thermal Conductivity, *Inorg. Chem.*, 61 (2022) 968.

2. Sweta Yadav, Subhendu Jana, Gopabandhu Panigrahi, Sairam K. Malladi, Manish K. Niranjana, and **Jai Prakash**, Five coordinated Mn in

$\text{Ba}_4\text{Mn}_2\text{Si}_2\text{Te}_9$: synthesis, crystal structure, physical properties, and electronic structure, *Dalton Trans.*, 51 (2022) 9265.

3. Mohd Ishtiyak, Subhendu Jana, R. Karthikeyan, M. Ramesh, Bikash Tripathy, Sairam K. Malladi, Manish K. Niranjana, and **Jai Prakash**, Syntheses of Five New Layered Quaternary Chalcogenides SrScCuSe_3 , SrScCuTe_3 , BaScCuSe_3 , BaScCuTe_3 , and BaScAgTe_3 : Crystal Structures, Thermoelectric Properties, and Electronic Structures, *Inorg. Chem. Front.*, 8 (2021) 4086.



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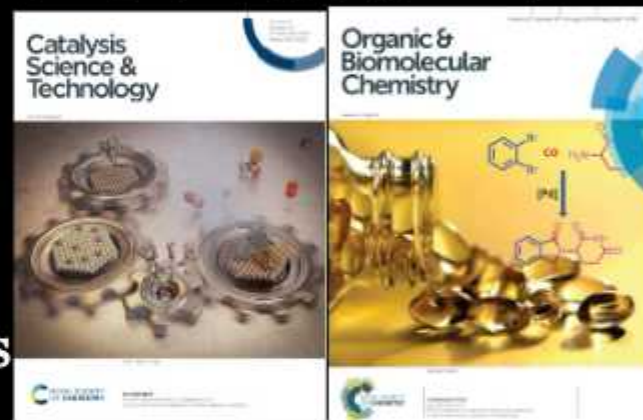


Major Areas of Research/Up to 3 major sponsored projects

- 1) Catalysis for Applied Organic Synthesis, Hydrogen generation, and Utilization
- 2) Hydrogenation of Arenes and Heteroarenes; Fine and Bulk chemicals (SERB)
- 3) Organofluorine and Pharmaceutical Chemistry

Major Research Facilities in the Group

- 1) Rotary Evaporators, LED lamps (Kessil)
- 2) High-pressure reactors
- 3) State-of-the-art lab ware for wet chemistry experiments



Technology/Product Developed/Up to 3 most significant Publications

- 1) R. Cauwenbergh, V. Goyal, R. Maiti, **K. Natte**,* S. Das, *Chem. Soc. Rev.*, 2022, 51, 9371-9423, Challenges and Recent Advancements in the Transformation of CO₂ to Carboxylic acids: Straightforward Assembly with homogeneous 3d Metals.
- 2) **K. Natte**, H. Neumann, M. Beller, R. V. Jagadeesh: *Angew Chem. Int. Ed.*, 2017, 56, 6384-6394, Catalytic Utilization of Methanol as a C1 Source in Chemical Synthesis
- 3) **K. Natte**, R. V. Jagadeesh, H. Neumann, M. Beller: *Nat. Commun*, 2017, 1344-1353, Convenient Reductive Aminations without Hydrogen: Selective Iron-catalyzed Synthesis of N-Methylamines



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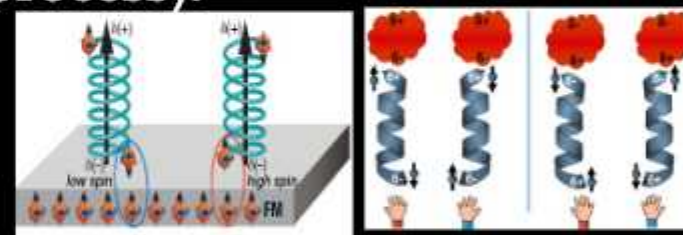
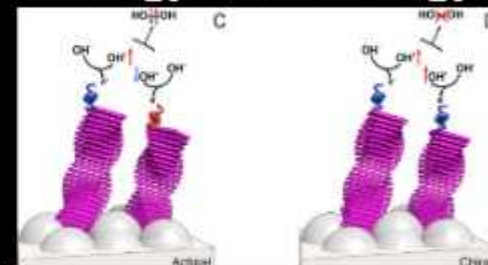


Major Areas of Research/Up to 3 major sponsored projects

1. Spin-dependent electrochemistry and its application in clean energy technology.
2. Surface chemistry and heterogeneous catalysis
3. Spin-controlled electron transfer through proteins

Major Research Facilities in the Group

1. Electrochemical workstation (Procurement is under process).
2. UV-VIS spectrophotometer (Procurement is under process).



Technology/Product Developed/Up to 3 most significant Publications

1. **Koyel Banerjee-Ghosh**, Oren Ben Dor, Francesco Tassinari, Eyal Capua, Shira Yochelis, Amir Capua, See-Hun Yang, Stuart Stephen Papworth Parkin, Soumyajit Sarkar, Leeor Kronik, Lech Tomasz Baczewski, Ron Naaman and Yossi Paltiel, "Separation of Enantiomers by Enantio-Specific Interaction of Chiral Molecules with Magnetic Substrates", *Science*, **360**, 2018, 1331–1334.
2. **Koyel Banerjee-Ghosh**, Shirsendu Ghosh, Hisham Mazal, Inbal Riven, Gilad Haran, Ron Naaman, "Long-range charge reorganization as an allosteric control signal in proteins", *J. Am. Chem. Soc.*, **142**, 2020, 20456–20462.
3. Wenyan Zhang, **Koyel Banerjee-Ghosh**, Francesco Tassinari, and Ron Naaman, "Enhanced Electrochemical Water Splitting with Chiral Molecule-Coated Fe_3O_4 Nanoparticles", *ACS Energy Lett.*, **3**, 2018,

2308–2313.



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Major Areas of Research/Up to 3 major sponsored projects

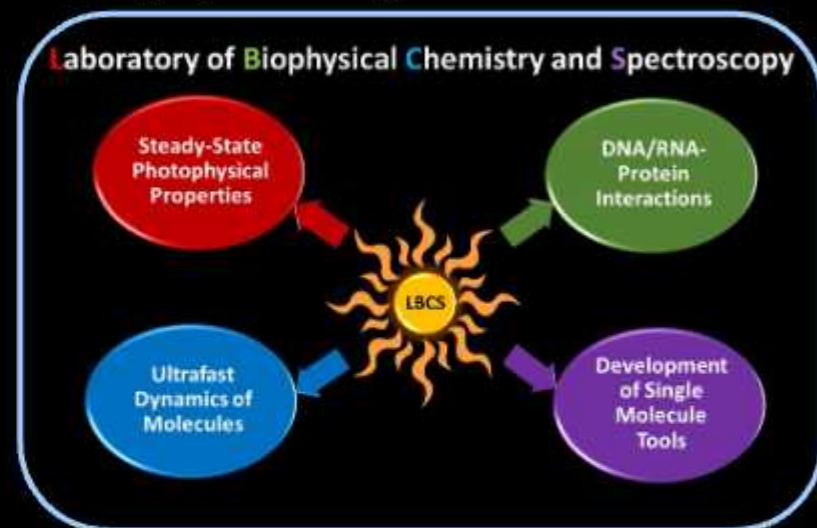
- 1) Exploring Protein-DNA, Drug-DNA and Drug-Protein Interactions Using Spectroscopic Tools (SERB-SRG)
- 2) Understanding Ultrafast Excited State Dynamics of Molecules
- 3) Development of Single Molecule Fluorescence Techniques

Major Research Facilities in the Group

- 1) UV-Visible Absorption Spectrophotometer
- 2) Steady-State Fluorescence Spectrophotometer
- 3) A Wet Lab to Perform Experiments
- 4) A Dry Lab for Processing the Data

Technology/Product Developed/Up to 3 most significant Publications

- 1) Sudhanshu Sharma, Dineshbabu Takkella, Pintu Kumar, Krishna Gavvala*
Spectroscopic Analysis to Identify the Binding Site for Rifampicin on Bovine Serum Albumin
Spectrochim. Acta. A. 2022, 283, 121721.
- 2) Dineshbabu Takkella, Sudhanshu Sharma, Lara Martinez-Fernandez*, Krishna Gavvala*
Excited-State Dynamics of Imiquimod in Aqueous Solutions
J. Photochem. Photobiol. A. 2022, 431, 113998.
- 3) Ruchika Bhujbalrao, Krishna Gavvala, Reman Kumar Singh, Juhi Singh, Christian Boudier, Sutapa Chakrabarti, G Naresh Patwari*, Yves Mély*, Ruchi Anand*
Identification of Allosteric Hotspots Regulating the Ribosomal RNA Binding by Antibiotic Resistance-Confering Erm Methyltransferases
J. Biol. Chem. 2022, 298, 102208.



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Major Areas of Research/Up to 3 major sponsored projects

Synthesis and Processing of 2D materials

Supercapacitors, Hybrid metal-ion capacitors

Multivalent metal-ion batteries; On-chip energy storage

Funding: SERB-DST

Major Research Facilities in the Group

Multi-channel Battery tester, electrochemical workstation

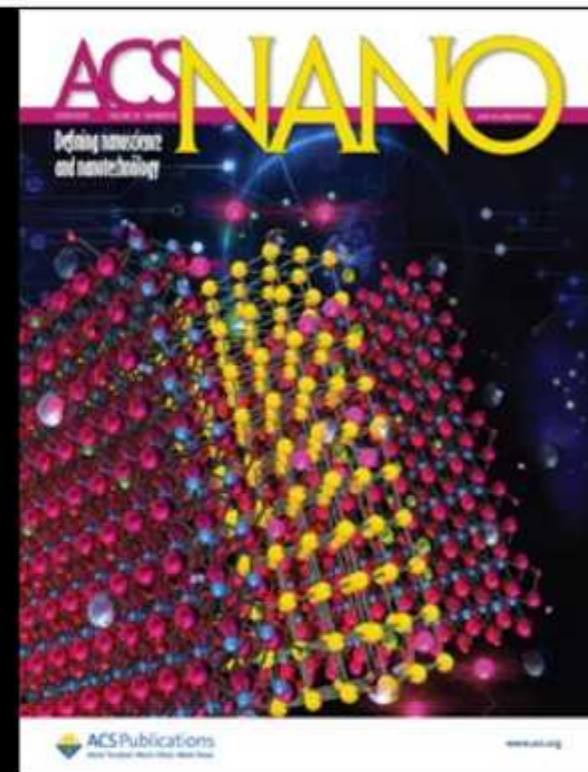
Glove box, Crimping/decrimping machine

Technology/Product Developed/Up to 3 most significant Publications

N. Kurra* et al., Journal of Energy Storage, 2022, 55, Part C, 105702.

N. Kurra* et al., Energy Storage Materials, 2021, 39, 347.

H. Saini et al., ACS Nano, 2021, 15, 18742.





Prabu Sankar Ganesan

Professor, Organometallics and Materials Chemistry Lab, Department of Chemistry

Phone No: +914023016256; Institute Email: prabu@chy.iith.ac.in; Webpage Link: <https://people.iith.ac.in/prabu/index.html>

Major Areas of Research

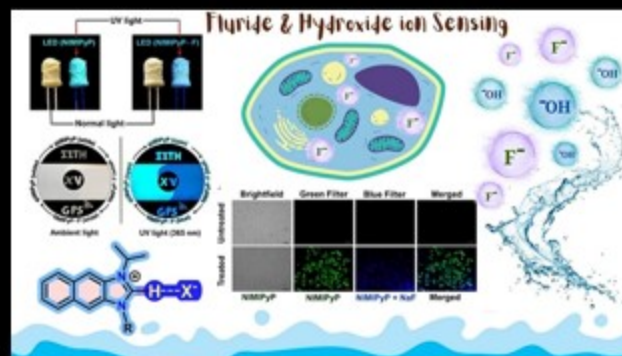
- ❖ Late Transition Metal Chemistry
- ❖ Heavier Main Group P-block Chemistry-Catalysis
- ❖ Light Emitting Molecules
- ❖ High Performance Light Weight Composite Materials
- ❖ Organometallic Official Molecules

Major Research Facilities in the Group

- ❖ MBraun Glove Box, UNILab
- ❖ GCMS-QP2010 Ultra
- ❖ JEOL ESR FA 200
- ❖ MBraun SPS
- ❖ SHIMADZU FTIR
- ❖ LABINDIA UV-vis
- ❖ IKA Electrasyn 2.0 Pro
- ❖ HITACHI FS F4700
- ❖ Bruker D8 VENTURE SCXRD
- ❖ SHIMADZU HPLC

Technology/Product Developed

- ❖ Fast Access to Phosphine Cu(I)-Carbene Complexes
- ❖ Organo Ru(II) Salts for Neurodegenerative/Neuromuscular Diseases
- ❖ d¹⁰ Light-Emitting Materials



Dr. M. Annadhasan

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Department of Chemistry

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Major Areas of Research/Up to 3 major sponsored projects

Crystals-based programmable photonic circuits.

Optically/electrically pumped microlasers.

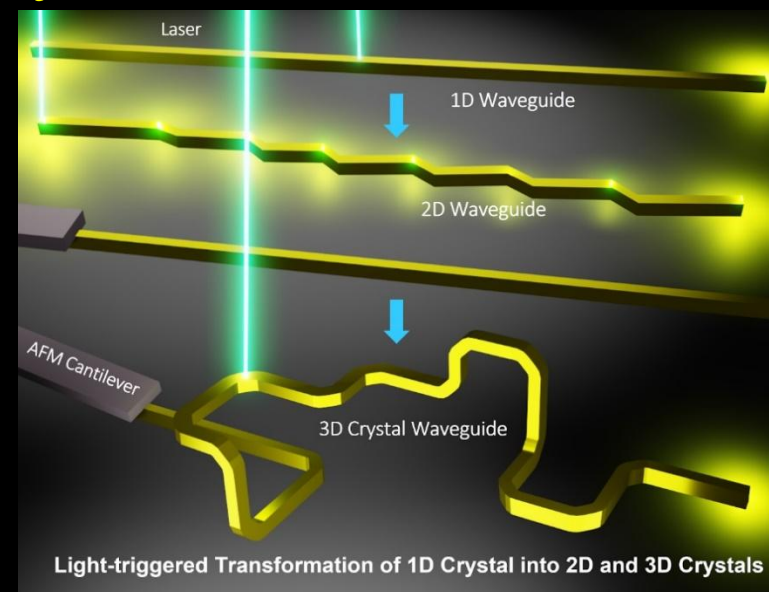
Bandwidth tunable Carbon dots.

Major Research Facilities in the Group

Fluorescence spectrophotometer (in process).

Laser for photonics studies (in process).

Synthesis lab with basic facilities and fume hoods



Technology/Product Developed/Up to 3 most significant Publications

1. *Highly Efficient Color-Tunable Organic Co-crystals Unveiling Polymorphism, Isomerism, Delayed Fluorescence for Optical Waveguides and Cell-imaging*, D. Barman, **M. Annadhasan**, A. Bidkar, P. Rajamalli, D. Barman, S. S. Ghosh*, R. Chandrasekar* & P. K. Iyer* **Nat. Commun.**, (2023) **14**, 6648.

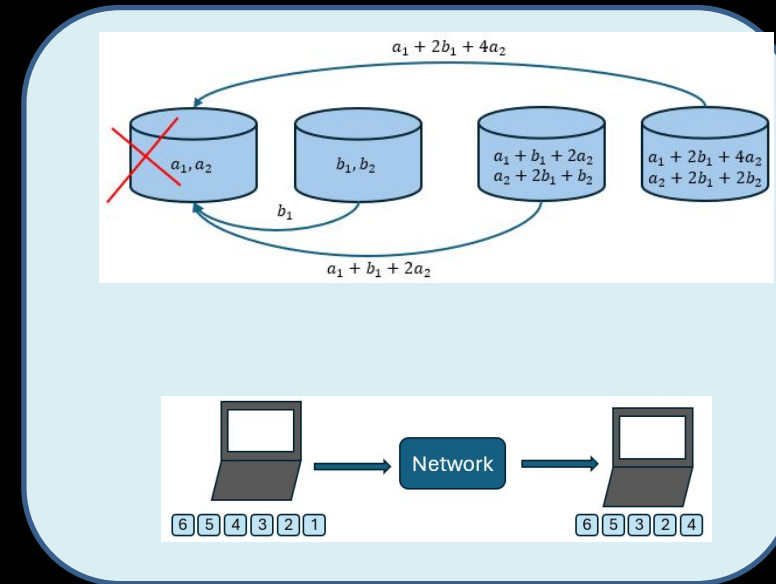
2. *Dimension Engineering of Stimuli-Responsive 1D Molecular Crystals into Unusual 2D and 3D Zigzag Waveguides*, **M. Annadhasan**, A. Vinod Kumar, S. Nandy, P. Giri, M. K. Panda, K. V. J. Jose*, R. Chandrasekar*, **Angew. Chem. Int. Ed.** (2023), **65**, e202302929.

3. *Mechanophotonics: Flexible Single-Crystal Organic Waveguides and Circuits*, **M. Annadhasan**, A. Agrawal, S. Bhunia, V. V. Pradeep, S. S. Zade*, C. M. Reddy*, R. Chandrasekar*, **Angew. Chem. Int. Ed.** (2020), **59**, 13852-13858.



Major Areas of Research/Up to 3 major sponsored projects

1. Codes for storage, privacy, streaming and communications
2. Design of communication systems and
3. Milli-meter wave communications



Technology/Product Developed/Up to 3 most significant Publications

1. Vajha et al., Clay Codes: Moulding {MDS} Codes to Yield an {MSR} Code, USENIX FAST 2018
2. Balaji, Krishnan, Vajha et al. Erasure coding for distributed storage: An overview, Science China Information Sciences, 2018.
3. Vajha et al. Explicit rate-optimal streaming codes with smaller field size, Transactions in Information Theory, 2023



Priyadarshi Chakraborty

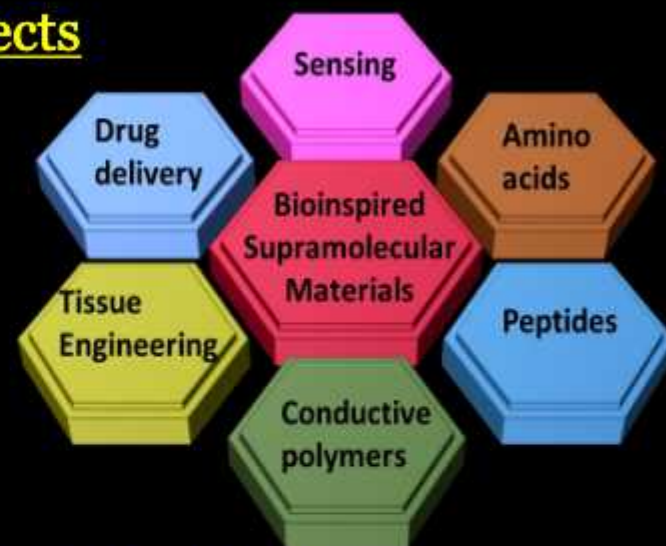
Assistant Professor, Bioinspired Supramolecular Materials Group, Department of Chemistry

Office Room No.: CHY-FO-19; Mobile :+91 9434616214, Email: priyadarshi@chy.iith.ac.in; Webpage: <https://priyadarshi9.wixsite.com/priyadarshi>

Major Areas of Research/Up to 3 major sponsored projects

Areas of Research: Self-assembly, Co-assembly, Hydrogels, Conductive polymers, tissue engineering, cell culture, drug delivery.

Sponsored projects: Ramalingaswami Grant (DBT) on Cardiac tissue engineering.



Major Research Facilities in the Group

Chemistry Department facilities including UV- Vis, FTIR, XRD, NMR, DSC.

Technology/Product Developed/Up to 3 most significant Publications

1. Nano-Engineered Peptide-Based Antimicrobial Conductive Supramolecular Biomaterial for Cardiac Tissue Engineering. P. Chakraborty, H. Oved, D. Bychenko, Y. Yao, Y. Tang, S. Zilberzwige-Tal, G. Wei, T. Dvir and E. Gazit, *Advanced Materials*, 2021, **33**, 2008715.
2. Unusual two-step assembly of a minimalistic dipeptide-based functional hypergelator. P. Chakraborty, Y. Tang, T. Yamamoto, Y. Yao, T. Guterman, S. Zilberzwige-Tal, N. Adadi, W. Ji, T. Dvir, A. Ramamoorthy, G. Wei, E. Gazit, *Advanced Materials* 2020, **32**, 1906043.
3. A Self-Healing, All-Organic, Conducting, Composite Peptide Hydrogel as Pressure Sensor and Electrogenic Cell Soft Substrate. P. Chakraborty, T. Guterman, N. Adadi, M. Yadid, T. Brosh, L. Adler-Abramovich, T. Dvir and E. Gazit, *ACS Nano* 2019, **13**, 163-175.





Gedu Satyanarayana

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Areas of Research:

Transition Metal Catalysis

Site Selective C–H Activation

Acid-Promoted Domino Processes

Electrochemical Organic Transformations

Lab facilities:

ElectraSyn 2.0

Microwave Synthesizer

Key publications:

1. Karu Ramesh, Gedu Satyanarayana. *Green Chem.*, **2018**, *20*, 369–374.
2. Perla Ramesh, Chinnabattigalla Sreenivasulu, Dakoju Ravi Kishore, Dasari Srinivas, Koteswara Rao Gorantla, Bhabani S. Mallik* and Gedu Satyanarayana*. *J. Org. Chem.* **2022**, *87*, 5, 2204–2221.
3. Dasari Srinivas, Gedu Satyanarayana. *Org. Lett.* **2021**, *23*, 19, 7353–7358.



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CHY-FI-518, 040-2301-6266.; 7330732020; sksingh@chy.iith.ac.in; <https://sites.google.com/view/skslab>



Major Areas of Research/Up to 3 major sponsored projects

Computational Exploration of Bonding and Covalency in Actinide Molecular Complexes (SERB-SRG)

Molecular Modeling of Spin-Vibronic Coupling and Magnetic Relaxation in Molecule-Based Magnets; Spin-Crossover Phenomenon

Computational Modelling of Catalytic Sites for Small Molecule Activations mediated by Transition Metal and Actinide Molecular Complexes and Metal-Organic Frameworks

Major Research Facilities in the Group

Tools for High-Level Relativistic DFT and Multiconfigurational Methods

In-house computing resource with ~ 4 nodes (~226 cores) with 192 GB RAM; One High-End Node (~56 core) with 768 GB RAM

Software Tools: Amsterdam Density Functional (ADF) Code, OpenMOLCAS, ORCA, VASP, SIESTA, Multiwfn, NBO

Technology/Product Developed/Up to 3 most significant Publications

P. Kumar, J. F. Gonzalez, P. P. Sahu, N. Ahmed, J. Acharya, V. Kumar, O. Cador, F. Pointillart, **Saurabh Kumar Singh***, V. Chandrasekhar*, "Magneto Caloric Effect and Slow Magnetic Relaxation in Peroxide-assisted Tetranuclear Lanthanide Assemblies" *Inorg. Chem. Front.* **2022**, 9, 5072-5092.

D. Shao*, S. Moorthy, Y. Zhou, Si-Tong Wu, J.-Y. Zhu, J. Yang, D.-Q. Wu*, **Saurabh Kumar Singh***, "Field-induced slow magnetic relaxation behaviours in binuclear cobalt(II) metallocycle and exchange-coupled cluster" *Dalton Trans.* **2022**, 51, 9357-9368.

D. Shao*, P. P.Sahu, W. J. Tang, Yang-Lu Zhang, Y. Zhou, X. Q. Wei*, Z. Tian*, **Saurabh Kumar Singh*** "A single-ion magnet building block strategy toward Dy₂ single-molecule magnets with enhanced magnetic performance" *Dalton Trans.* **2022**, 51, 18610-18621.



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Indian Institute of Technology Hyderabad



Sivakumar Vaidyanathan,

Associate Professor, APEL, Department of Chemistry

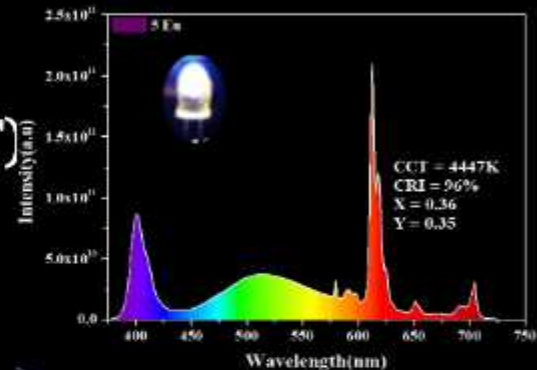
5th Floor, #17.; Office Phone No.; Mobile (9438503635); Institute Email; vsiva@chy.iith.ac.in

Major Areas of Research/Up to 3 major sponsored projects

Luminescence Lanthanide complexes for smart lightings (DST)

Luminophores for organic light emitting diodes (SERB)

Phosphors for solid state lightings (including NIR emitters)

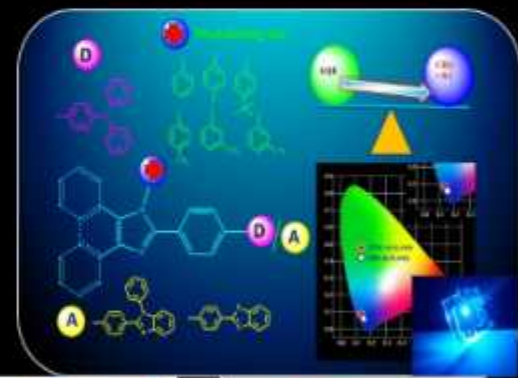
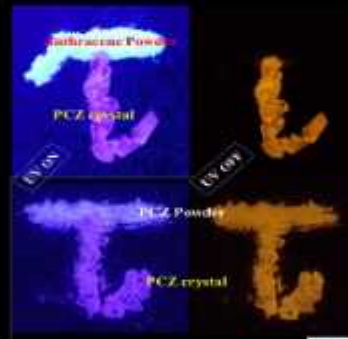


Major Research Facilities in the Group

Spectrofluorometer

Optical study – in film form

Electrochemical systems

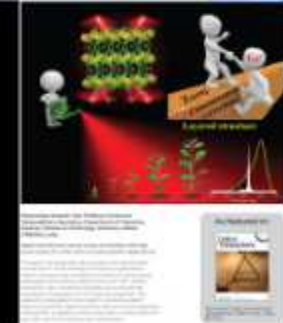


Technology/Product Developed/Up to 3 most significant Publications

Efficient TADF yellow emitter for OLEDs

White phosphors for solid state lightings

Room temp phosphorescence organic dyes



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Major Areas of Research/Up to 3 major sponsored projects

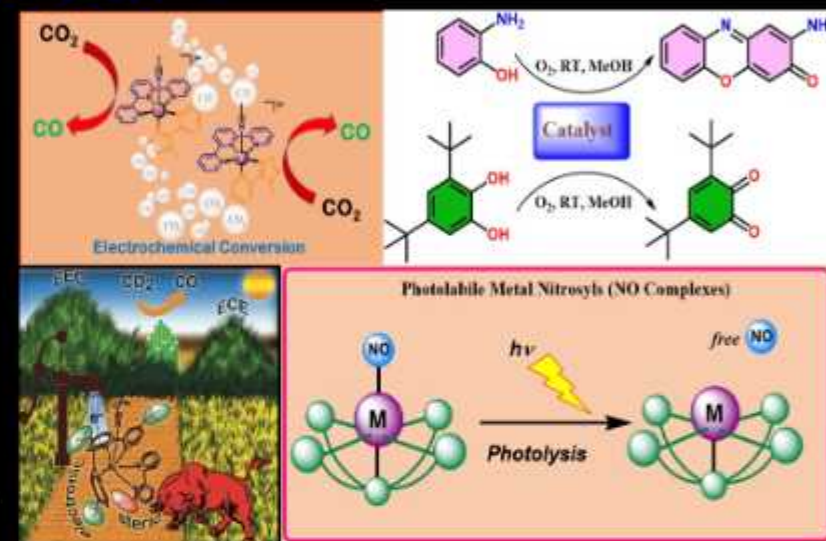
- 1) Bioinspired Catalysts for Solar fuel Production:
Photochemical WOC/ Proton Reduction/ CO₂ Reduction
- 2) Designed Photoactive Ruthenium Nitrosyls for
Site-specific NO Delivery
- 3) Mimicking Catechol Oxidase and Phenoxazinone
Synthase Activity/ DNA binding / DNA Cleavage
/ Anti-Cancer Activity

Major Research Facilities in the Group

- 1) Electrochemical setup/Spectro-electrochemical set up
- 2) UV-vis Spectrometer
- 3) Oxygraph Instrument for measuring dissolved O₂ /Cryogenic set up for
low temperature reaction

Technology/Product Developed/Up to 3 most significant Publications

- 1) Tetrazole-Substituted Isomeric Ruthenium Polypyridyl Complexes for Low Overpotential Electrocatalytic CO₂ Reduction
B. Giri, A. Mahata, T. Kella, D. Shee, F. D. Angelis, S. Maji *J. Catal.*, **2022**, *405*, 15-23.
- 2) Design, Synthesis, Structural, Spectral, and Redox Properties and Phenoxazinone Synthase Activity of Tripodal
Pentacoordinate
Mn(II) Complexes with Impressive Turnover Numbers
S. Kumbhakar, B. Giri, A. Muley, K. S. Karumban, S. Maji *Dalton Trans.*, **2021**, *50*, 16601-16612.
- 3) Near-IR Light-Induced Photorelease of Nitric Oxide (NO) on Ruthenium Nitrosyl Complexes: Formation, Reactivity, and
Biological
Effects
B. Giri, T. Saini, S. Kumbhakar, K. S. K, A. Muley, A. Misra, S. Maji *Dalton Trans.*, **2020**, *49*, 10772 – 10785.





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Major Areas of Research/Up to 3 major sponsored projects

Heterogeneous catalysis

Biomass conversion

C-N bond construction

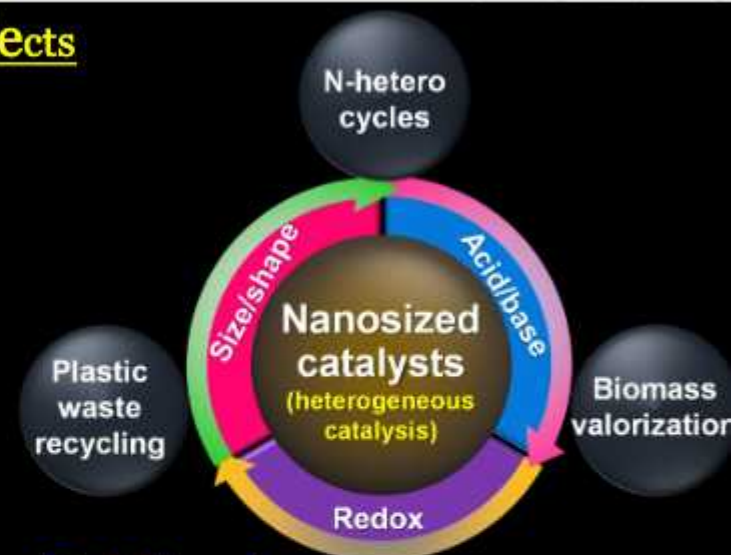
Plastic waste recycling

Major Research Facilities in the Group

GC

Centrifuge

Technology/Product Developed/Up to 3 most significant Publications



1. N. S. Bhat, S. L. Hegde, S. Dutta,* P. Sudarsanam*. Efficient synthesis of 5 (hydroxymethyl)furfural esters from polymeric carbohydrates using 5 (chloromethyl)furfural as a reactive intermediate, ACS Sustainable Chemistry & Engineering 10 (2022) 5803–5809.
2. P. Sudarsanam,* A. Köckritz, H. Atia, M.H. Amin, A. Brückner*. Synergistic nanostructured MnO_x/TiO₂ catalyst for highly selective synthesis of aromatic imines. ChemCatChem 13 (2021) 1990-1997.
3. P. Sudarsanam,* E. Peeters, E.V. Makshina, V.I. Parvulescu, B.F. Sels*. Advances in porous and nanoscale catalysts for viable biomass conversion. Chemical Society 2421.



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Surajit Maity

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Major Areas of Research

Excited State Photophysical Processes of Isolated Microsolvated Molecules

Spectroscopic characterization of molecular docking on the surface of biomolecular prototypes

Electronic Structure and Properties of Isolated Metal Complexes in the Gas Phase

Major Research Facilities in the Group

Molecular Beam Machine equipped with LIF, DF, TOF-Mass spectrometer set-up

UV-VIS/ IR OPO (200-4000 nm, 1 cm⁻¹ resolution, ns-pulsed laser system)

Laser ablation set-up for molecular reaction under plasma conditions

Technology/Product Developed/Up to 3 most significant Publications

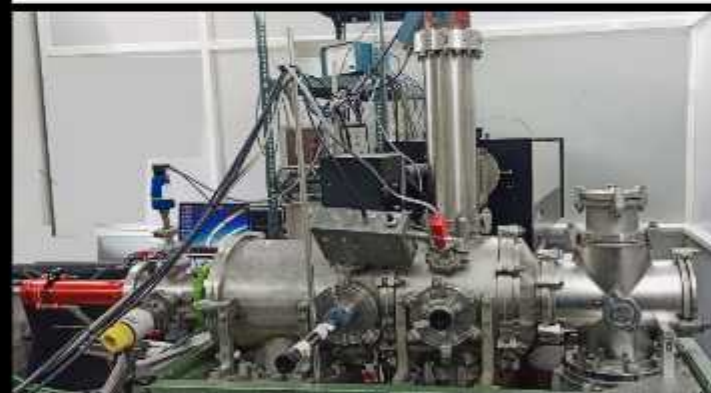
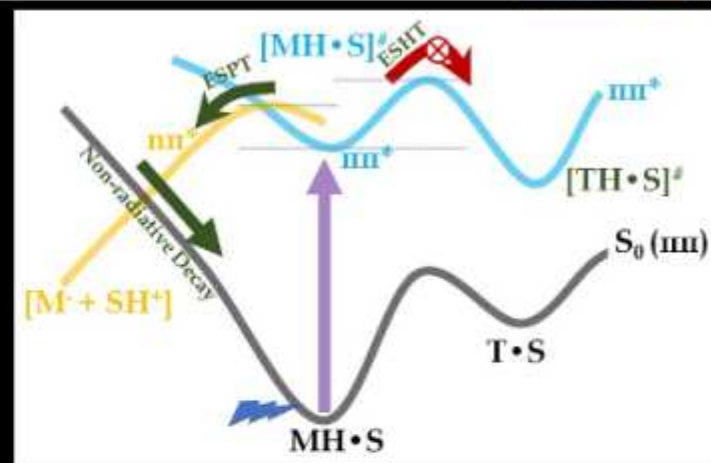
Developed methodologies to measure excited state energy barriers spectroscopically

Demonstrate method to quantitatively describe the kinetic isotope effect upon state-specific electronic excitation

S. Khodia, Ramesh J. and S. Maity, Phys. Chem. Chem. Phys., 2022, doi.org/10.1039/D2CP04676H

S. Khodia and S. Maity, Phys. Chem. Chem. Phys., 2022,24, 12043-12051; doi.org/10.1039/D2CP01121B

S. Baweja, P. Roy Chowdhury, S. Maity, Spectrochim. Acta A: Mol. Biomol. Spectros. 2022, 265, 120386





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Major Areas of Research

- High energy, less/No cobalt Lithium-ion batteries.
- Sodium ion batteries.
- Dual- carbon (metal-free) batteries.
- Li-ion, Lead-carbon hybrid ultracapacitors
- Recycling Li-ion batteries.

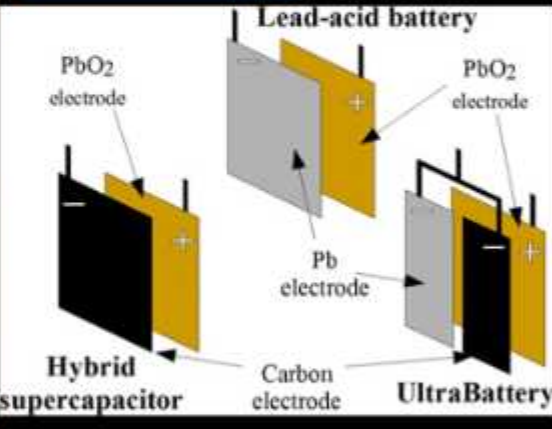
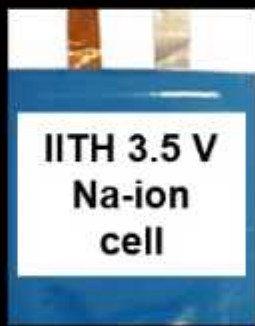
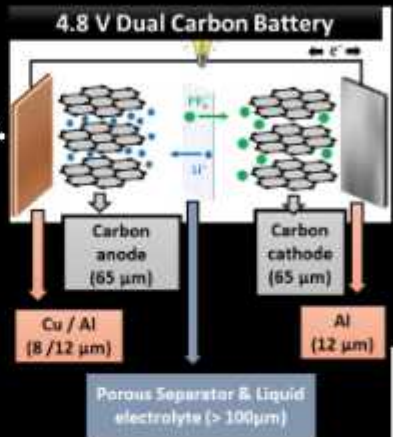
Major Research Facilities in the Group

- Glove boxes for coin cell and pouch cell assembly.
- Battery cyclers, potentiostats and galvanostats.
- Pouch cell assembly (partially).
- Material synthesis apparatus.

Technology/Product Developed/Up to 3 most significant Publications

1. LMR-NMC cathodes and Si-C anodes for High energy, Lithium-ion batteries.
2. 4.8 V Dual- carbon metal free batteries.
3. 2.75 V, 14 Wh kg⁻¹ Li-ion hybrid ultracapacitors.
4. Cost-effective hydrometallurgical processes for Recycling Li-ion batteries.

Ref. *Advanced Energy Materials*, 2100135 (2021), *ACS Sustainable Chem. Eng.* 2022,10, 23, 7515.





Prof. Tarun K. Panda

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Department of Chemistry

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Major Areas of Research

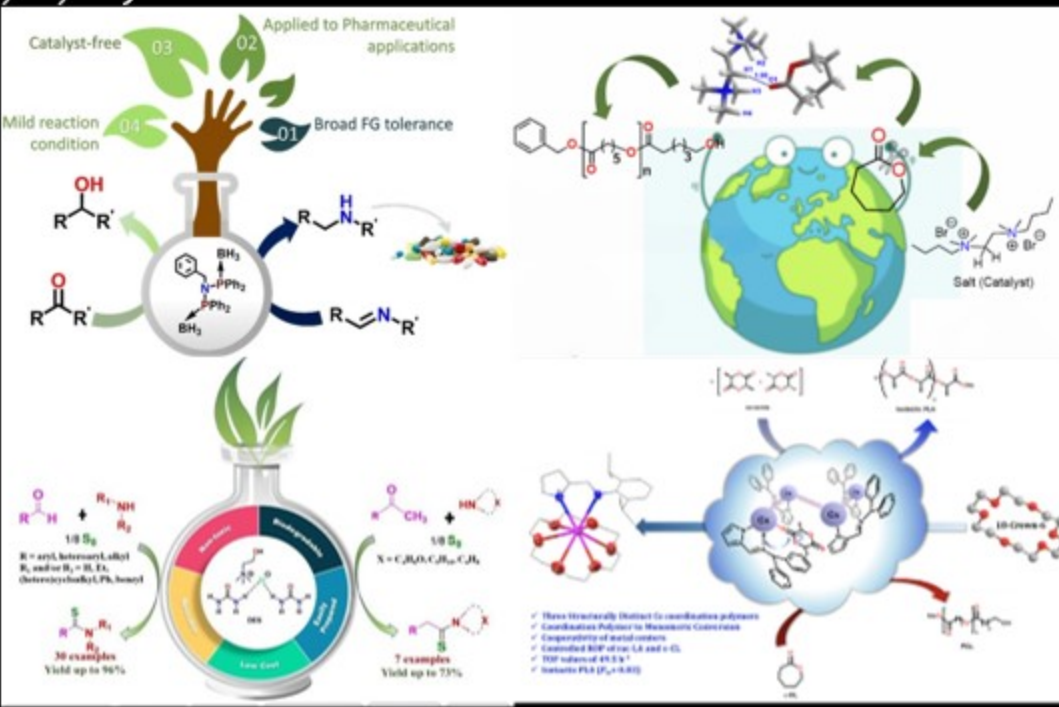
- 1) Synthesis and Application of various organo-earth abundant metal complexes
- 2) Atom-efficient catalytic C-X (X = N, O, S, P, C, B, Si) bondformation using earth-abundant catalysts
- 3) Ring opening Polymerization (ROP) of cyclic esters and amides using earth-abundant metal catalysts

Major Research Facilities in the Group

- MBRAUN Glove Box Workstations
- Gel Permeation Chromatography (GPC) System
- High-Pressure Reactor

Technology/Product Developed

- 1) Green synthesis of poly ϵ -caprolactone using a metal-free catalyst via non-covalent interaction, *Green Chem.*, 2025, 27, 527-534.
- 2) Amidophosphine Boranes as Hydroboration Reagents for Nitriles, Alkynes, and Carboxylic Acids, *Organic Letters*, 2023, 25, 43, 7923-7927.
- 3) Ligand Mediated Metal-Metal and Ligand-Metal Cooperativity in Cesium Coordination Polymers. Efficient ROP Catalysis of Cyclic Esters, *Chem. Eur. J.* 2025, e202501304.



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Department of Chemistry

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Webpage Link: <https://kvrao-group.webnode.page>



Major Areas of Research/Up to 3 major sponsored projects

Supramolecular polymers; Porous organic polymers; Soft-materials
Organic semiconductors

Major Research Facilities in the Group

UV-Vis-NIR spectrometer with temperature control (-10 to 100 °C)
Fluorescence spectrometer
Microwave synthesizer



Technology/Product Developed/Up to 3 most significant Publications

1. Post-synthetic π -extension of perylene conjugated porous polymer via APEX reactions: tunable optical and gas storage properties,
DS Ingle, AC Yadav, K Kumari, SKK Singh, DJ Babu, KV Rao
Chem. Commun. DOI: 10.1039/D2CC05340C
2. Supramolecular depolymerization in the mixture of two poor solvents: mechanistic insights and modulation of supramolecular polymerization of ionic π -systems
S Kotha, MFJ Mabesoone, D Srideep, R Sahu, SK Reddy, KV Rao
Angew. Chem., Int. Ed., **2021**, *60*, 5459
3. Synthesis and Self-assembly of Benzoperylene Benzimidazoles: Tunable Morphology with Aggregation-Induced Enhanced Emission
D Srideep, K Sriram, S Kotha, DJ Babu, SK Singh, KV Rao
Chem. – Asian J., **2022**, *17*, e202200099



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