Abhijit Sau

Assistant Professor, Glycochemistry Research Lab, Department of Chemistr

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Major Areas of Research/Up to 3 major sponsored projects

- 1) Development of synthetic stagey 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) o°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

Assistant Professor, Computational Modelling of Advanced Materials Laboratory, , Department of Chemistry

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Major Areas of Research/Up to 3 major sponsored projects

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 <complex-block>

1. A. H. Proppe, A. Johnston, S. Teale, <u>Arup Mahata</u>, 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. <u>Arup Mahata</u>,* 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, <u>Arup Mahata</u>, 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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Major Areas of Research/Up to 3 major sponsored projects

- 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 sulphoxidation 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 judicially positioned metal ion toward aerobic sulphoxidation. Mouli and Mishra, RSC Adv., 2022, 12, 3990







Dr. Bhabani Shankar Mallik

Professor, Advanced Computing Lab, Department of Chemistry

Institute Email: bhabani@chy.iith.ac.in; Webpage Link

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**). RESEARCH

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

MATERIALS SCIENCE

Autonomous self-repair in piezoelectric molecular crystals

భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్ भारतीय प्रौद्योगिकी संस्थान हैदराबाद Indian Institute of Technology Hyderabad

Surojit Bhunia^{1,2}, Shubham Chandel³⁺, Sumanta Kumar Karan⁴, Somnath Dey⁵, Akash Tiwari³, Susobhan Das¹, Nishkarsh Kumar³, Rituparno Chowdhurv¹, Saikat Mondal^{1,2}, Ishita Ghosh¹, Amit Mondal¹, Bhanu Bhusan Khatua⁴, Nirmalya Ghosh³*, 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







Science

REPORT

Debasish Koner

Assistant Professor, Dynamics & ML Lab, Department of Chemistry

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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 Ar₂H⁺ 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, Photosupercapacitors

Major Research Facilities in the Group: Class

AAA Solar Simulator, IPCE Meaurement facility, UV-Vis, Fluoresence 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

Organic Synthesis Lab, Department of Chemistry

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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

Major Research Facilities in the Group



Flash Chromatography Multivial Reactor

Direct α -Benzylation of Methyl Enol Ethers with Activated Benzyl Alcohols: Its Rearrangement and Access to (±)-

Tetrahydronyasol, Propterol A, and 1,3-Diarylpropane J. Org. Chem. 2019, 84, 21, 14270-14280. (DOI:

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: <u>10.1016/j.bmcl.2021.127883</u>

Solvent controlled synthesis of 2,3-diarylepoxy indenones and α-hydroxy diarylindanones and their evaluation as inhibitors of DNA alkylation repair *Org. Biomol. Chem.*, **2022**, 20, 5820-5835. DOI: <u>10.1039/D2OB00595F</u>

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





Jai Prakash

Associate Professor, Department of Chemistry

Chem Build. .; Email: jaiprakash@chy.iith.ac.in; webpage: https://jai-group.webnode.page/

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. Niranjan, and **Jai Prakash**,

Germanium Antimony Bonding in $Ba_4Ge_2Sb_2Te_{10}$ with Low Thermal Conductivity, *Inorg. Chem.*, 61 (2022) 968.

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

Ba4Mn2Si2Te9: 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. Niranjan, and Jai Prakash, Syntheses of Five New Layered Quaternary Chalcogenides SrScCuSe₃, SrScCuTe₃, BaScCuSe₃,

BaScCuTe₃, and BaScAgTe₃: Crystal Structures, Thermoelectric Properties, and Electronic Structures, *Inorg. Chem. Front.*, 8 (2021) 4086.









Kishore Natte

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CHE S20 ; Office Phone No.; Mobile 9121562367; kishore.natte@chy.iith.ac.in ; Kishore Natte | IIT Hyderabad

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

R. Cauwenbergh, V. Goyal, R. Maiti, <u>K. Natte</u>,* 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.
 <u>K.Natte</u>, 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
 <u>K. Natte</u>, R.V.Jagadeesh, H.Neumann, M.Beller: Nat. Commun, 2017,1344-1353, Convenient Reductive Aminations without Hydrogen: Selective Iron-catalyzed Synthesis of N-Methylamines



Organic & Biomolecular Chemistry

Koyel Banerjee Ghosh

Assistant Professor, Chiral Materials & Electronics (CME), Chemistry

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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). <u>Technology/Product Developed/Up to 3 most</u> <u>significant Publications</u>

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. <u>Koyel Banerjee-Ghosh</u>, Shirsendu Ghosh, Hisham Mazal, Inbal Riven, Gilad Haran, Ron Naaman, "Long-range charge reorganization as an allosteric control signal in proteins", <u>J. Am. Chem. Soc</u>, 142, 2020, 20456–20462.
- **3.** Wenyan Zhang, <u>Koyel Banerjee-Ghosh</u>, Francesco Tassinari, and Ron Naaman, "Enhanced Electrochemical Water Splitting with Chiral Molecule-Coated Fe₃O₄ Nanoparticles", <u>ACS Energy Lett</u>., **3**, 2018,

2308–2313.









Krishna Gavvala

Assistant Professor, Biophysical Chemistry Lab, Department of Chemistry

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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



- 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-
- **Conferring Erm**
 - Methyltransferases
 - J. Biol. Chem. 2022, 298, 102208.





Narendra Kurra

Assistant Professor, Electrochem Mater Lab, Department of Chemistry

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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.







Ganesan Prabu Sankar

Professor, Organometallics and Materials Chemistry Lab, Department of Chemistry

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Major Areas of Research/Up to 3 major sponsored projects

-N-Heterocyclic Carbenes (NHC) -Cu, Ni, Co, Pd, Au, Ru, Zn-NHC Catalysts -Bismuth Catalysts -C-S Cross-Coupling Reactions & Click Chemistry

Major Research Facilities in the Group

GC-MS, Fluorescence spectrometer (VT, solid-state & Solution state), UVvis spectrometer, Cyclic Voltammetry, Glove Box, Solvent Purification System, ESR & SXRD

Technology/Product Developed/Up to 3 most significant Publications

Chemistry-An Asian Journal, 2022, 17(18), e202200594. Catalysis Letter 2022, 1-11. Chemistry-An Asian Journal, 2023, 18, asia.202201138.



Cu(II) Catalyst

Highly Active



Triazole Methyl Carbazole

- Excellent Yield

6:32 min

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, <u>M. Annadhasan</u>, 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, <u>M. Annadhasan</u>, A. Agrawal, S. Bhunia, V. V. Pradeep, S. S. Zade^{*}, C. M. Reddy^{*}, R. Chandrasekar^{*}, *Angew. Chem. Int. Ed.* (2020), 59, 13852-13858.

Asst. Professor, Smart Materials & Nano-Photonics Lab, Department of Chemistry

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Myna Vajha

Assistant Professor, Codes and Communication Systems, 22

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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

<u>Technology/Product Developed/Up to 3 most</u> <u>significant Publications</u>

- 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

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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

Professor, Synthetic Organic Lab, Department of Chemistry

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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.







Saurabh Kumar Singh

Assistant Professor, CICG, Department of Chemistry

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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.

 Modeling Spin-States

 Modeling Spin-States

 Nodeling Spin-States

 New Generation Magnetic Material

 New Generation Magnetic Material

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.





Sivakumar Vaidyanathan,

Associate Professor, APEL, Department of Chemistry

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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











Somnath Maji

Associate Professor, BioInspired Catalysis, Department of Chemistry

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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
- 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
- Oxygraph Instrument for measuring dissolved O₂ /Cryogenic set up for low temperature reaction



Technology/Product Developed/Up to 3 most significant Publications

- 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.
- 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.

 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 <u>Major Research Facilities in the Group</u>

Nanosized catalysts (heterogeneous catalysis)

Redox

Indian Institute of Technology Hyderabad

Plastic

waste

recycling

N-hetero

cycles

Biomass valorization

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/TiO_2 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.

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.



भारतीय प्रौद्योगिकी संस्थान हैदराबाद Indian Institute of Technology Hyderabad



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Major Areas of Research/Up to 3 major sponsored projects

- 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) bond
- formation 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 **Mass Spectrometer High-Pressure Reactor**





Indian Institute of Technology Hyderabad

Technology/Product Developed/Up to 3 most significant Publications

1) J. Bhattacharjee, A. Sarkar and T. K. Panda, The Chemical Record, Alkali and Alkaline Earth Metal Complexes as Versatile Catalysts for Ring-Opening Polymerization of Cyclic Esters, 2021, 21, 1898-1911.

2) Harinath, J. Bhattacharjee, and T. K. Panda, Facile Reduction of Carboxylic Acids to Primary Alcohols under Metal-free and Solvent-free Conditions, Chemical Communications, 2019, 55, 1386-1389.

3) J. Bhattacharjee, A. Harinath, I. Banerjee, H. P. Nayek and T. K. Panda, Highly Active Dinuclear Ti^{IV} Complexes for Catalytic Formation of Carbon -భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్ Heteroatom Bond, Inorg. Chem., 2018, 57, 12610-12623. भारतीय प्रौद्योगिकी संस्थान हैदराबाद



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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





