Chemistry@BIT

✓Interdisciplinary Chemical Sciences

✓Education & Research

✓Discovery and Excellence

Vision

*To become a recognized center of **excellence for teaching**, **research and innovations** and make significant contribution for producing academic professionals and entrepreneurs in frontier area of chemical sciences.*

Mission

- *To impart **quality education and fundamental concepts** of chemical sciences to students & scholars through our **state of art laboratory**, teaching and research facilities*
- *Building a scientific environment and motivation towards **innovation with quality research** in chemical sciences and interdisciplinary areas*

Dr. Ashoke Sharon, Professor & Head

Department of Chemistry
Birla Institute of Technology, Mesra, Ranchi

A DST-FIST Supported Department

Current FACULTY MEMBERS

Physical

Organic

InOrganic

2021: New Recruitments and Initiatives

Physical

Organic-Inorganic Hybrid Semiconductors for Electronic Applications, viz. Solar Cell, LED, FED, Photodiode

Dr. Debdutta Chakraborty

Computational Quantum Chemistry and Quantum Trajectories, Chemical Reaction Dynamics, Chemical Kinetics

Organic

Dr. Anirban Pradhan

Carbon Resources: Energy and Electronics:
synthesis of graphene, carbon nanoribbons (CNRs), poly aromatic hydrocarbons (PAHs), porous carbon materials: optoelectronics

InOrganic

Dr. Atul Kumar

Supramolecular chemistry, Self-assembly and Self-sorting, Host-guest chemistry, Catalysis Light harvesting systems, Photo-luminescent materials, Explosive Sensing Material

COURSES OFFERED :
& New Initiatives

- M.Sc. in CHEMISTRY
- Integrated MSc (I.M.Sc.)
- Ph.D.

- **6 Months Industrial Internship to 6 M.Sc. Students with Stipend at Dr. Reddy Lab, Hyderabad.**
- **MO21 Internship Project Training Given to 12 External Students (St Xavier College, Ranchi, 4th Sem M.Sc. Students)**

1	Vishal Singh	PHD/AC/10001/21	*IRF*
2	Mehak Bansal	PHD/AC/10002/21	*IRF*
3	Dev Brat Banerjee	PHD/AC/10003/21	
4	Leen Priya	PHD/AC/10004/21	
5	Raxita Pilania	PHD/AC/10005/21	
6	Anindita Mukherjee	PHD/AC/10051/20	*IRF*
7	Siddharth Parida	PHD/AC/10009/20	
8	MANSI SRIVASTAVA	PHD/AC/10003/20	
9	Md.Adnan Khan	PHD/AC/10006/20	
10	Avinash Singh	PHD/AC/10004/20	
11	Anurag Jaiswal	PHD/AC/10053/20	
12	BIPIN KUMAR SINGH	PHD/AC/10010/20	*IRF*
13	ADYA JHA	PHD/AC/10005/20	
14	SADHANA KUNDU	PHD/AC/10001/20	*IRF*
15	AYUSH ARYAN	PHD/AC/10007/20	*IRF*
16	Anuradha Mahanty	PHD/AC/10051/19	*IRF*
17	NEHA KUMARI	PHD/AC/10001/19	
18	UTTAM Kr MISHRA	PHD/AC/10052/19	*IRF*
19	Sahanwaj Khan	PHD/AC/10002/18	
20	NISHA KUMARI	PHD/AC/10051/18	
21	RAJAN KUMAR	PHD/AC/10001/18	
22	ANURAG MEHTA	PHD/AC/10003/18	
23	NIRGAMAN BAGE	PHD/AC/10051/17	
24	Saumya Shalu	PhD/AC/10001/16	
25	Amulya Prasad Panda	PHD/AC/10051/16	

Department BOS: A New Initiatives

Sr. No.	Name of the Member	Designation	Role
1	Dr. Ashoke Sharon	Professor, HOD (Ex-Officio)	Chairman
2	Dr. P.K. Srivastava	Professor	Internal Member
3	Dr. Usha Jha	Professor	Internal Member
4	Dr. J.P. Pandey	Professor	Internal Member
5	Dr. Sumit Mishra	Associate Professor	Internal Member
6	Dr. Subhendu Naskar	Associate Professor	Internal Member
7	Dr. P. Kar	Associate Professor	Internal Member
8	Dr. C. Bal	Associate Professor	Internal Member
9	Dr. G. Sen	Assistant Professor	Internal Member
10	**Dr. T. Ghose**	**Professor**	Internal Member
11	**Dr. Sudip Das**	**Professor**	Internal Member
12	**Dr. Pradyut Ghosh**	**Professor, IACS, Kolkata**	External Member
13	**Dr. Manas K. Ghorai**	**Professor, IIT Kanpur**	External Member
14	**Prof. Satish Patil**	**Professor, IISc Bangalore**	External Member
15	**Dr. Rakeshwar Bandichhor**	**Vice President, Dr. Reddy's Lab, Hyderabad**	External Member

HIGHLIGHTS

- Patents: 4 (One is PCT); Book Chapter: 26; Publications: **Last 5 Years: 71;**
- Ongoing: 3 Project (SERB, AICTE-TEQIP CRS and DBT)
- Approx. 30 Extramural Project Completed Successfully.
- DST FIST (400 MHz NMR and Computational Chemistry Lab)
- Consultancy from Dr. Reddy Lab, Hyderabad and Institute of Molecular and Cellular Biology, Singapore (A*Institute)Consultancy.
- International Collaboration: Kagoshima University Collaboration and Yearly Grant Release Since 2016 to continue Research Collaborative Work.
- Industry Collaboration: GVK Bioscience (Research Collaboration, Joint PhD Completed), Hyderabad, Dr. Reddy Lab Hyderabad (Academic, Consultancy, Internship), OTRIV Q3 Ahmedabad (Drug Delivery, Formulation and Analytics)

Education and Translation

TASMANION

Victoria University of Wellington

Shalini Divya · 1st

Co-founder and Chief Technology Officer at TasmanIon

Wellington, Wellington Region, New Zealand · Contact info

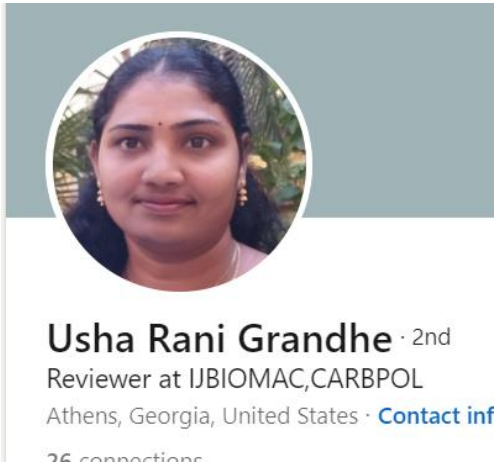
Department Alumni

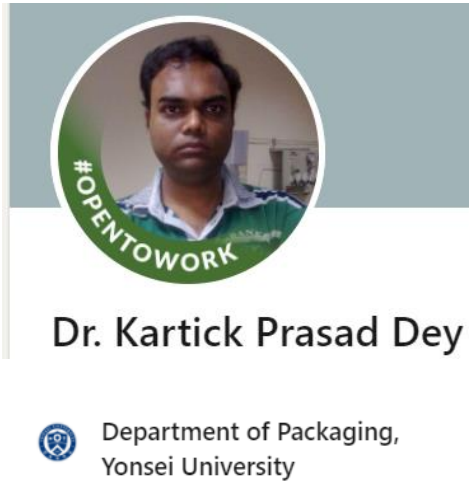
Dr. Konreddy Anand
Postdoctoral Associate
UGA, USA

Dr. Mohan Kasula
SERB NPDF: IIT Guwahati
Assistant Professor, BIHAR

Dr. Nandkishore
ICAR Scientist: IINRG, Ranchi
IPNI Scholar Award (2017)
USD 2000.

Dr. Tuniki Balaraju
GROUP LEADER, Aragen Biosciences, Hyderabad





Department Alumni

Dr. Arijit Hazari
M.Sc. Chemistry 2010-12
Current Position:
Postdoctoral Research Associate
(Marie Skłodowska-Curie fellow)
Institute of Inorganic Chemistry
University of Stuttgart, Germany

Dr. Shalini Divya
M.Sc. Chemistry 2013-15
Current Position:
Co-founder and Chief Technology Officer
TasmanIon, Wellington, New Zealand

Monika Yadav
I.M.Sc. Chemistry (2011-16)
Current Position:
Graduate Research Assistant
Department Of Chemistry
Purdue University, USA

Rahul Jha
B.Sc. Chemistry (2013-16)
Current Position:
Graduate Research Assistant
University of Kentucky, USA

Department Alumni

Shambhu Deo Chnadra
I.M.Sc. Chemistry (2013-18)
Current Position:
Graduate Research Assistant
Department Of Chemistry
The University of British Columbia,CANADA

Shrikant Singh
I.M.Sc. Chemistry (2013-18)
Current Position:
Graduate Research Assistant
Department Of Chemistry
University of Saskatchewan, CANADA

Simran
I.M.Sc. Chemistry (2013-18)
Current Position:
Graduate Research Assistant
Department Of Chemistry,
Graduate Research Assistant
Simon Fraser University British Columbia

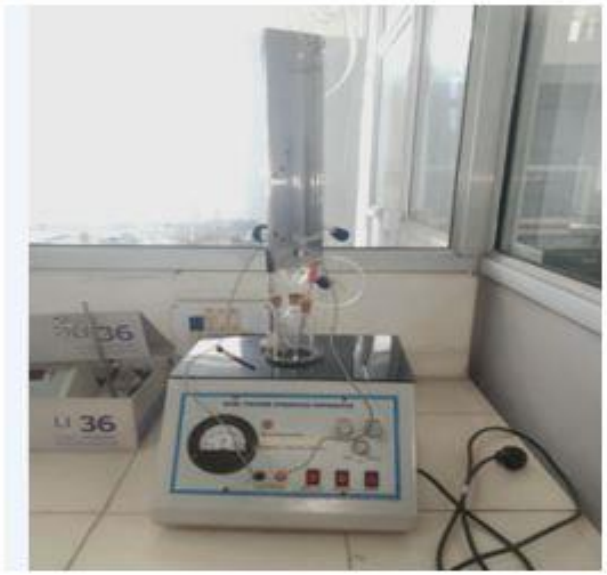
Major RESEARCH AREA:

- Medicinal Chemistry, & Drug Design
- Computation Chemistry & Molecular modelling
- Biomaterial Research
  - ❖Modified biomaterials in water treatment,
  - ❖ As controlled release matrices.
  - ❖Biocompatible Implants
- Environmental Chemistry, Water Remediation (Technology as Affordable System for Society)
- Polymer Chemistry: Polymer Matrix Composites (PMCs), Nanocomposites, Conducting Polymer, Bio & Gas Sensor application.
- Renewable Energy: Artificial Photosynthesis, Catalytic water oxidation and hydrogen evolution
- Organic-Inorganic Electronics
- Bioinorganic chemistry
- Electrochemistry, photo electrochemistry, electrochemical supercapacitor
- Non-linear Dynamics, chemical oscillations, fuels

New Grant Proposal under Evaluation

1. Electrocatalytic Hydrogen Evolution by Earth abundant transition metal based catalysts - Combine Homogeneous and Heterogeneous Approach: **SERB-CRG**
2. Transition metal based Hybrid Photoelectrochemical Cell for production of Solar fuel: SERB-SUPRA.
3. Influence of functionalization on the selective colorimetric sensing of anionic contaminants in water by gold nanoparticles, SERB, May-June 2021, 41 Lakhs
4. Inorganic arsenic sensing and removal by structured polyaminophenol, **CSIR**, Nov.-Dec. 2020, 41.96 Lakhs
5. Intelligent ammonia sensing device based on polym-aminophenol silver nanocomposite for environmental monitoring and medical diagnostic application, Aug-Sept 2020, 44.51 Lakhs, **DST**.
6. Application of MOFs and Electrocogulation for Water Treatment. **SERB-DST** under Evaluation.
7. Natural Product Inspired Synthesis and Biological Evaluation of Novel Pyranone/Pyridinone Analogs as Enhancer of Muscle Energy Expenditure to Treat Type 2 Diabetes. **SERB**, Submitted and under Evaluation

MAJOR INSTRUMENTAL FACILITIES at Department



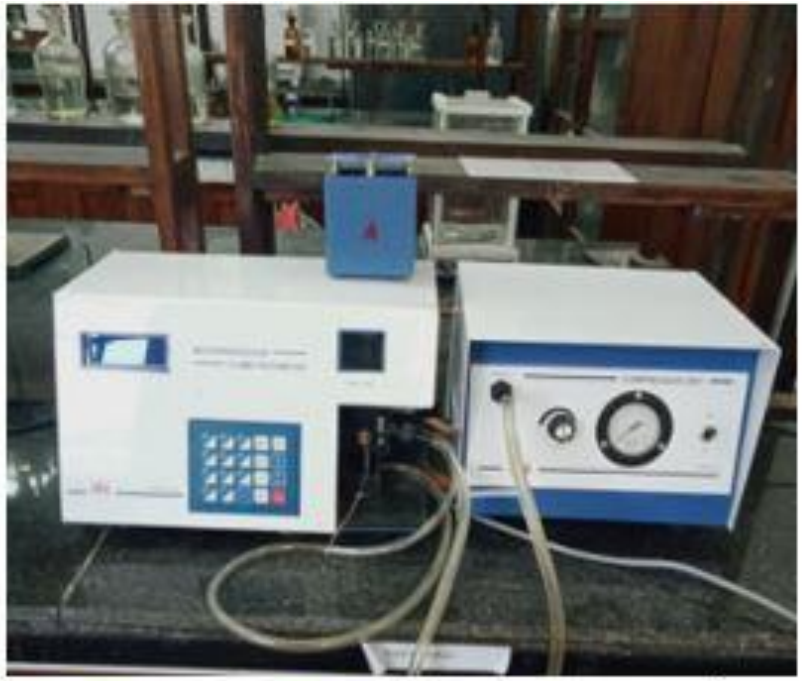
KARL FISCHER
TITRATION Apparatus

Osmometer

MAJOR INSTRUMENTAL FACILITIES at Department

MAJOR INSTRUMENTAL FACILITIES at Department

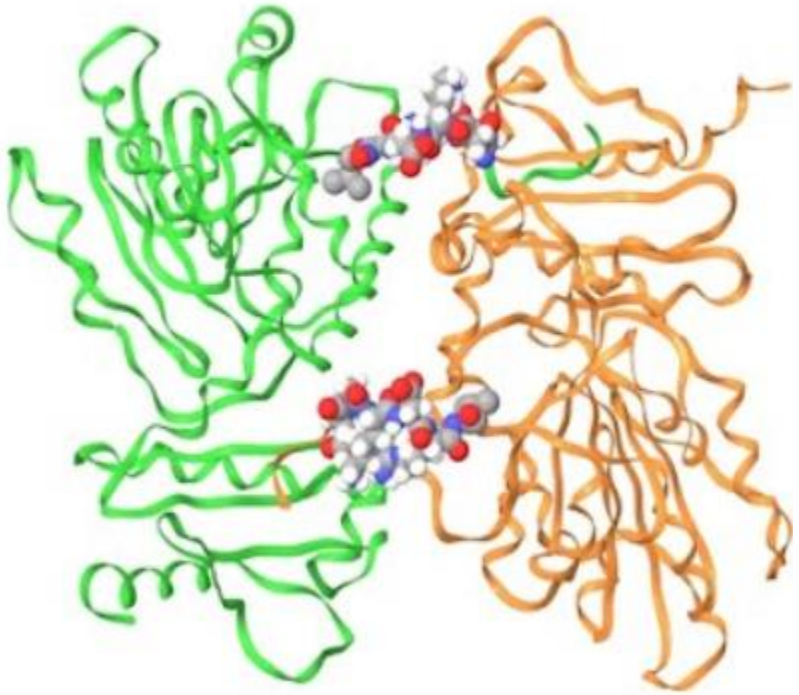
MAJOR INSTRUMENTAL FACILITIES at Department



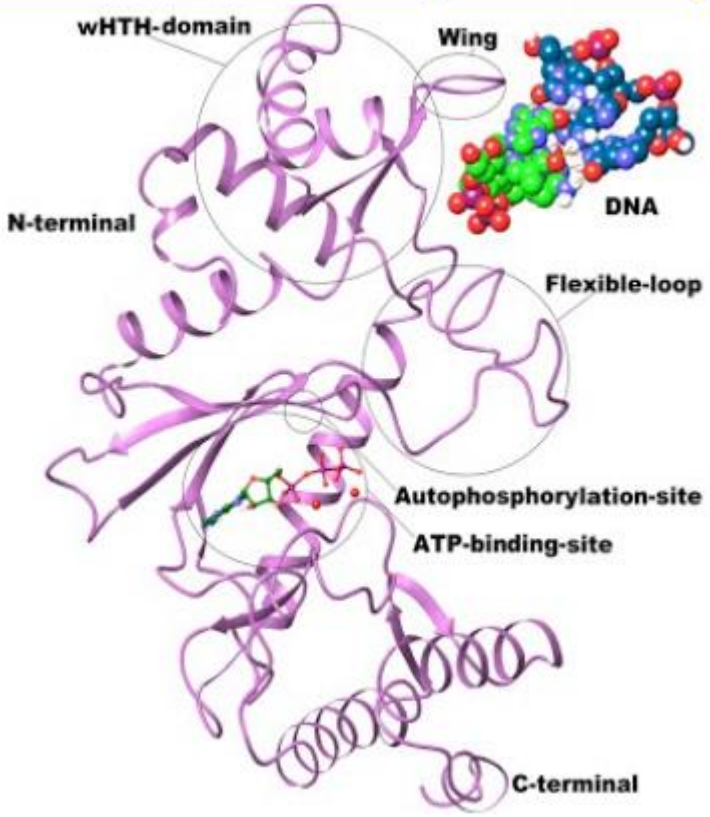
Flame Photometer

Departmental Research Activity

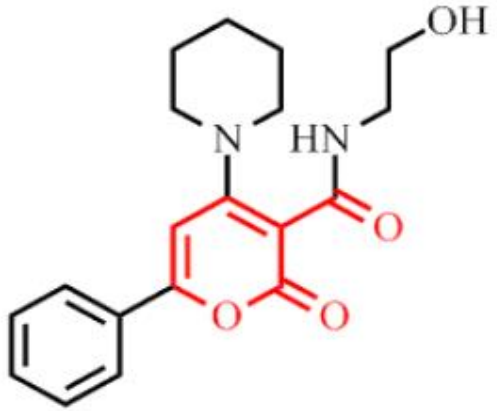
Structural Chemistry of Biology



Molecular Modeling and Design

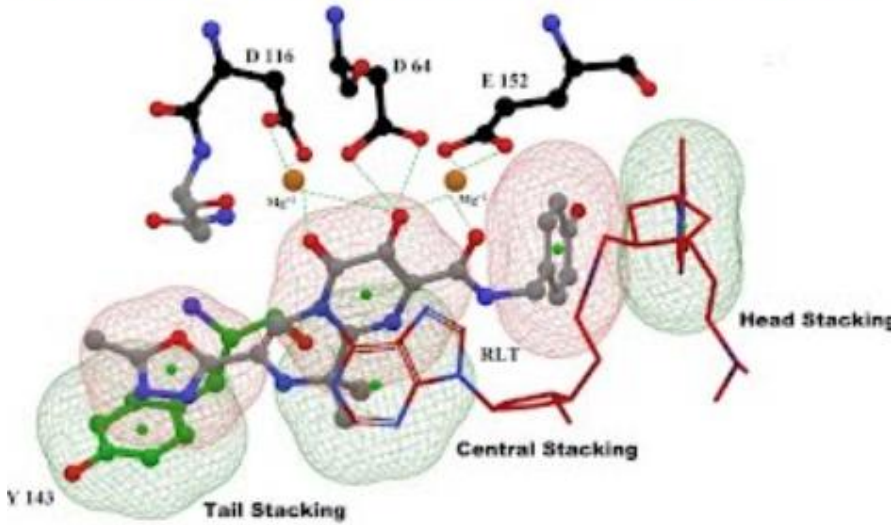


Organic-Medicinal Chemistry



NON-NUCLEOSIDE ANTIVIRALS

Pyranone Carboxamide Scaffold Exploration



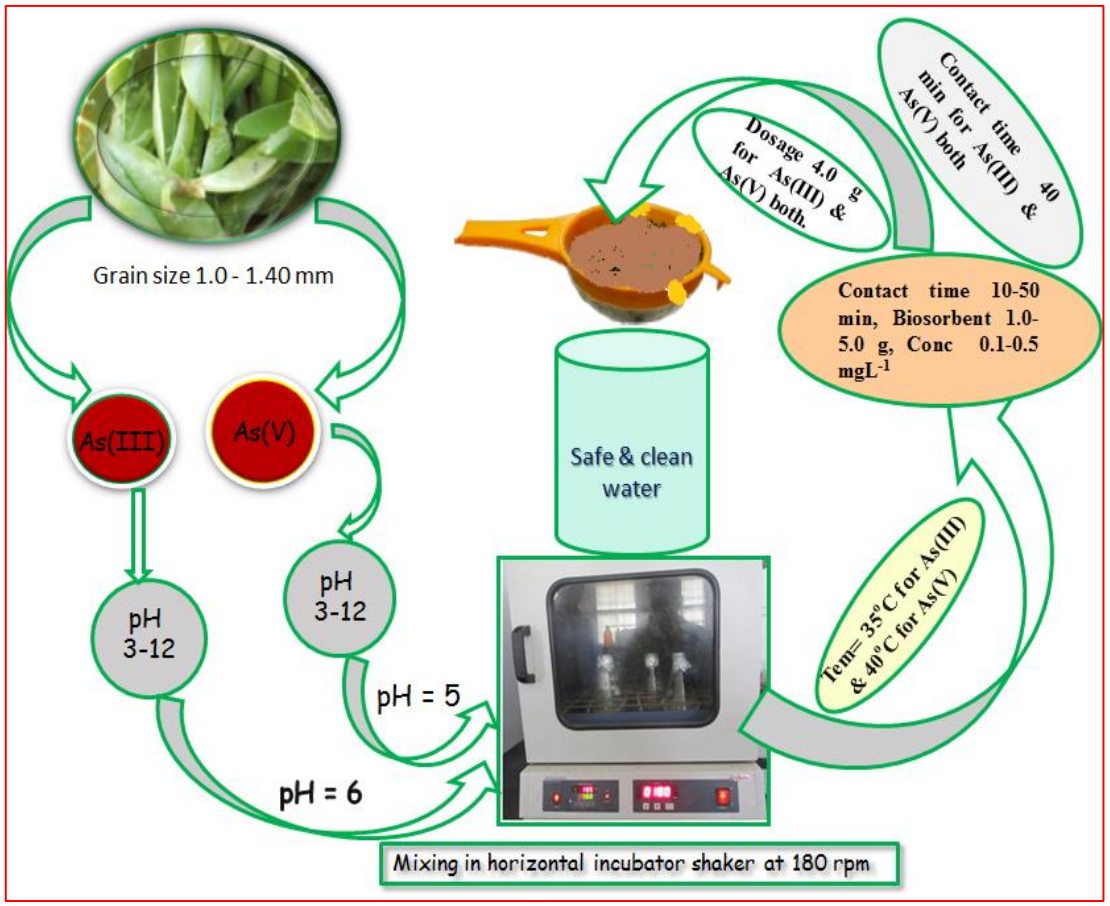
RALTEGRAVIR TRIPLE STACKING

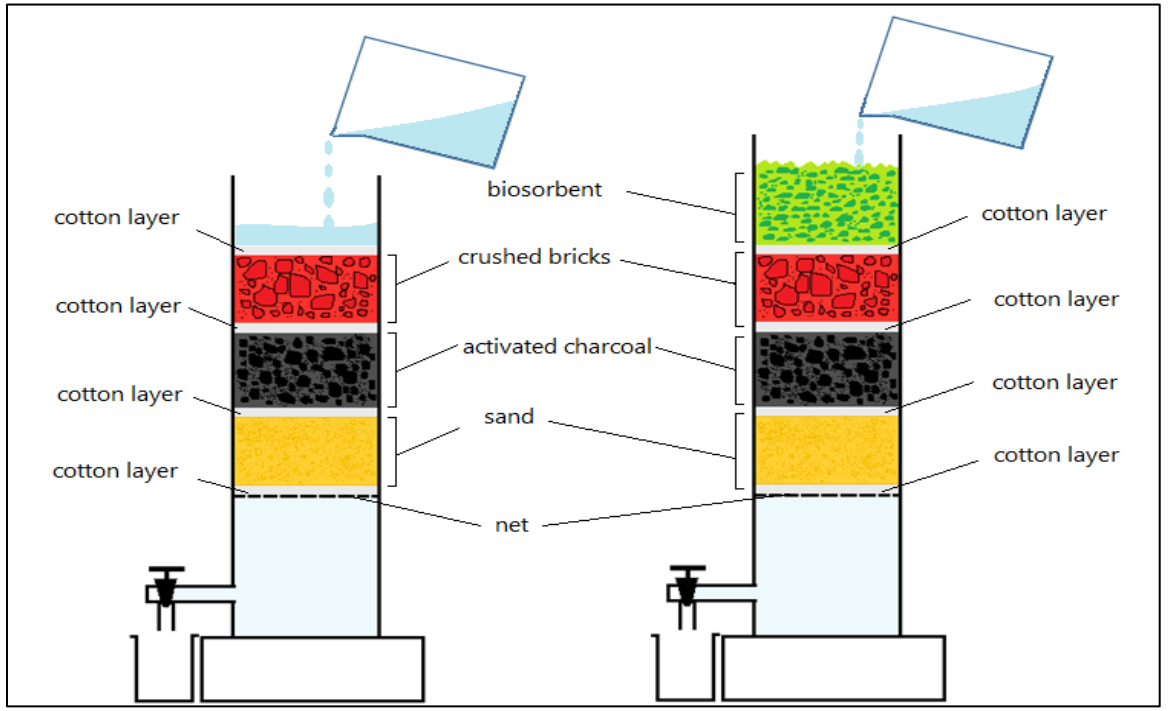
Synthesis and application of modified biopolymers

- Our department have a long history of research in modification of biopolymers (*polysaccharides* and *proteins*) *tailor-made* towards specific cutting edge applications.
- Microwave based eco-friendly methods of synthesis of graft copolymers namely *microwave initiated synthesis* (using microwave radiation alone to initiate grafting) and *microwave assisted synthesis* (a synergism of microwave radiation and chemical free radical initiator to initiate grafting) were developed in our department.
- The applications investigated for the synthesized novel grafted and cross-linked products are as follows:

Departmental Research Activity

Departmental Research Activity

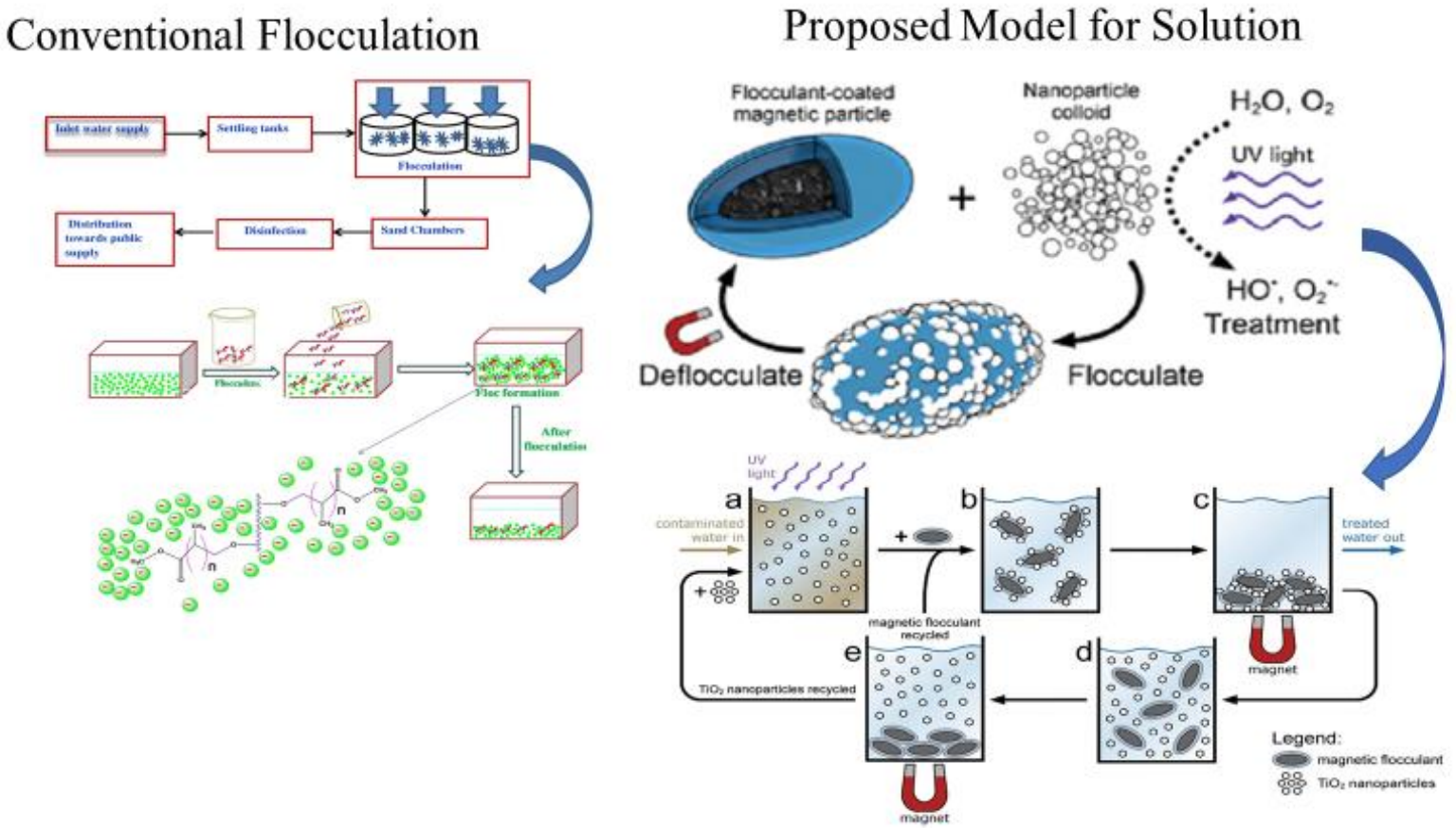


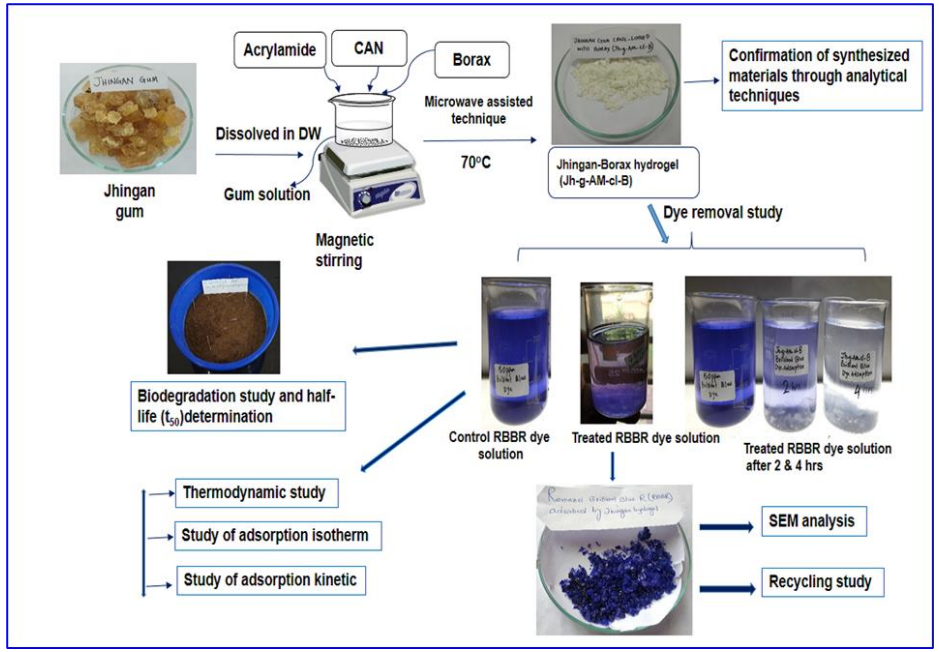


Departmental Research Activity

Research Area: Applications of modified biomaterials in water treatment, controlled release matrices and development of novel materials

Research Objective: Develop a complete solution for water treatment



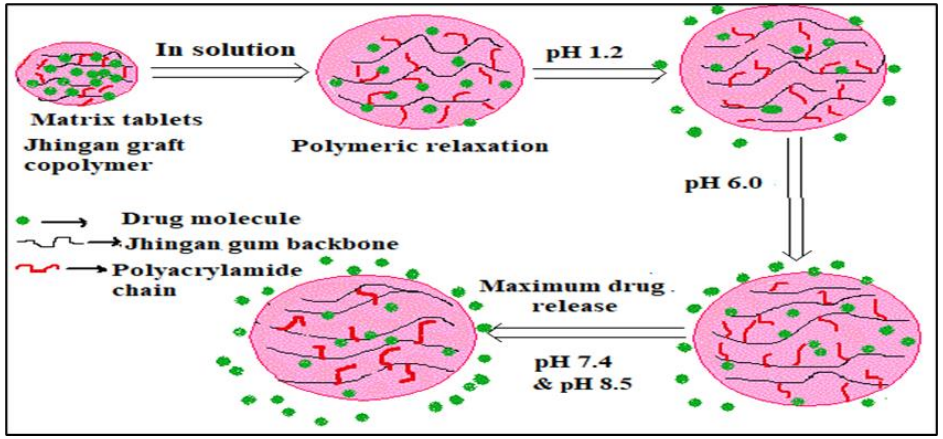


Dye removal studies:
International Journal of Biological Macromolecules 151 (2020) 677–690.

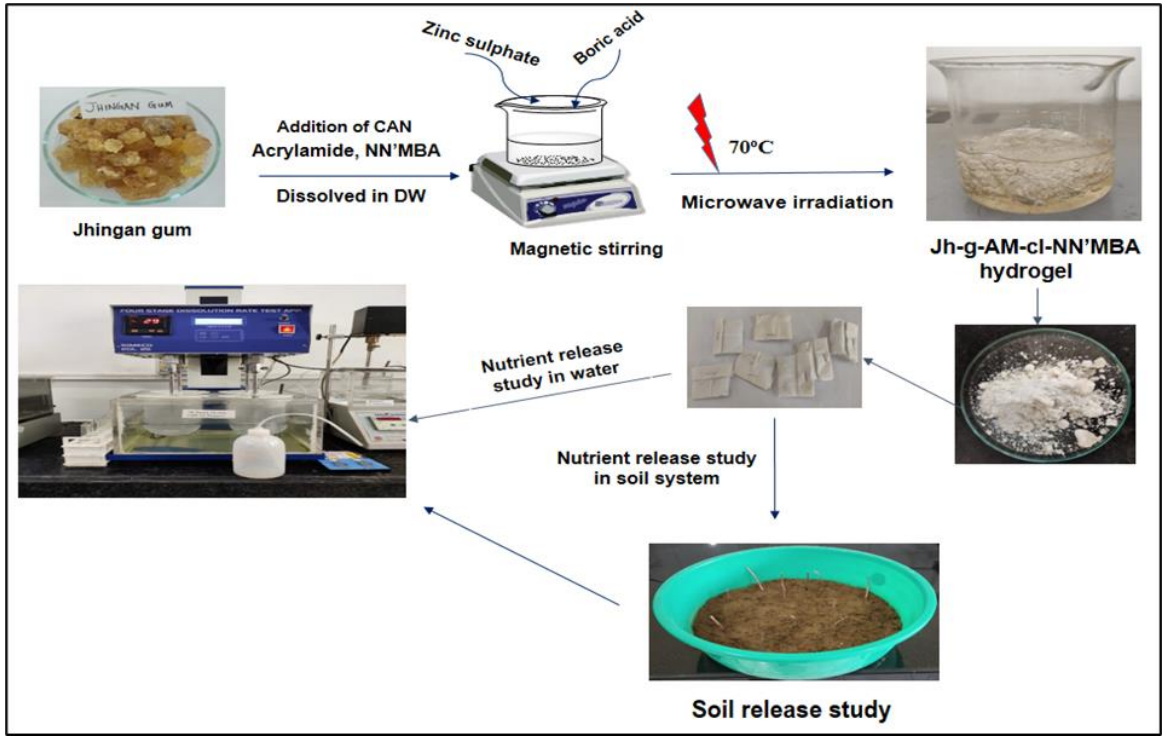
Water treatment: Present and Future; Using Magnetic flocculants & MOFs

Departmental Research Activity

Controlled release Studies for drugs and agricultural nutrients



Drug release studies: **International Journal of Biological Macromolecules 149 (2020) 908–920.**



Nutrient release studies: to be communicated soon

Future Prospects:

1. Release of nutrients, pesticides in controlled release mode to prevent environmental contamination
2. Drug release using microspheres
3. Development of adhesives and bioadhesives

Ongoing studies on developed adhesive

Departmental Research Activity

Extramural research grants as PI:

Completed:

1. UGC grant no: F.No 39.800/2010 (SR) 2011-14 **Rs 9,44,538**
2. DST grant no.: GOI 08/12-09141(2012-2015 **Rs 27,92, 389**
3. AICTE grant no.:8-207/RPS/1/2015-18 **Rs 14,11,765**

Sanctioned:

1. Jharkhand Council of Science and Technology, 2017 (Sanctioned) **Rs 5,00,000**

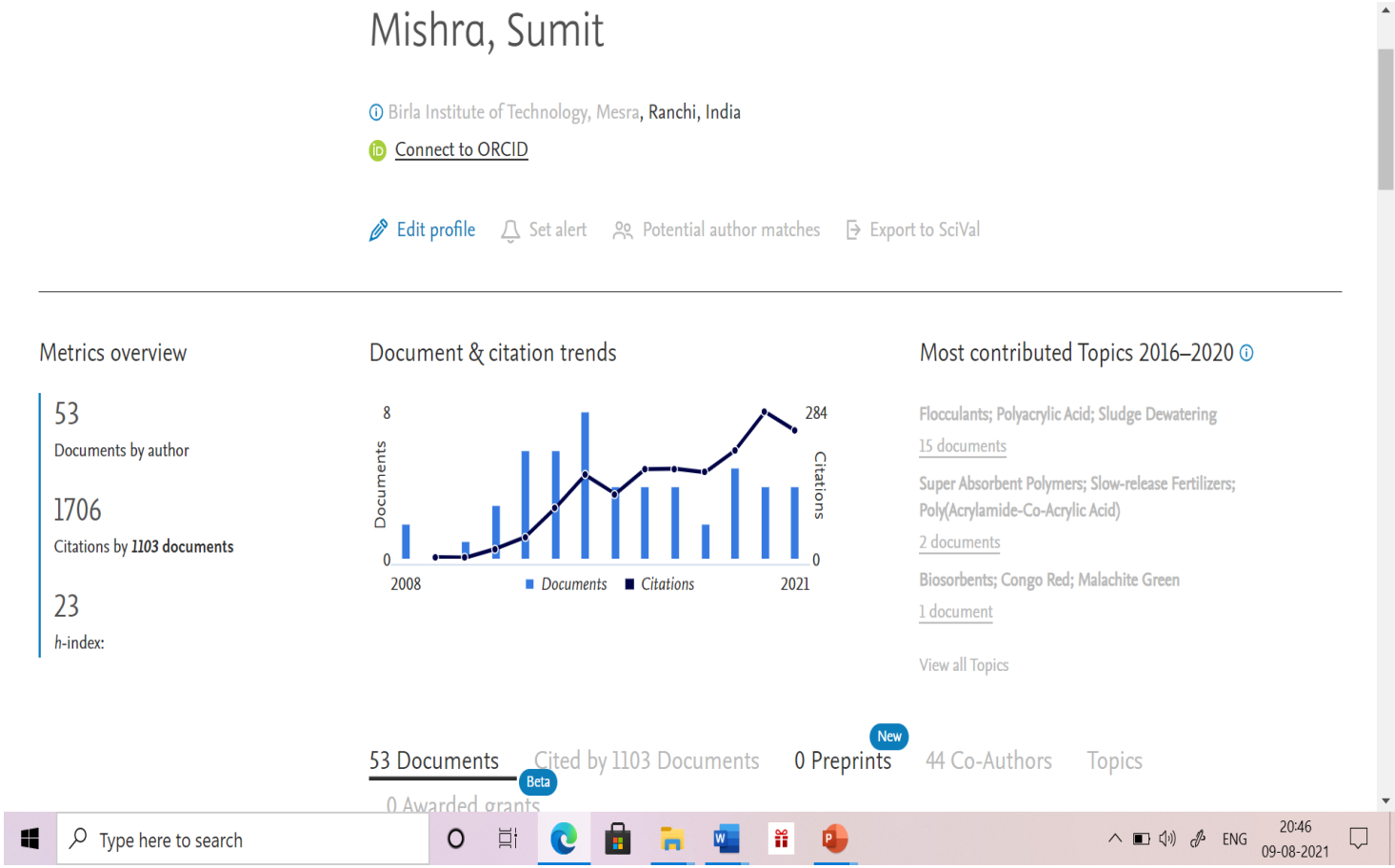
Pedagogy projects:

1. As Co-coordinator in Course preparation of Environmental Science under NMEICT project, Govt. of India. 10,00,000 INR

Total: 66,48, 692

Grants applied:

1. Core Research grant, SERB, 2021



H index: 23, Citation: 1706 (Scopus),

IF range: 1.8 to 9.38(present)

Publications: 53, Book Chapters:10

PhD students awarded: 5 (as guide), 3 (as co guide)

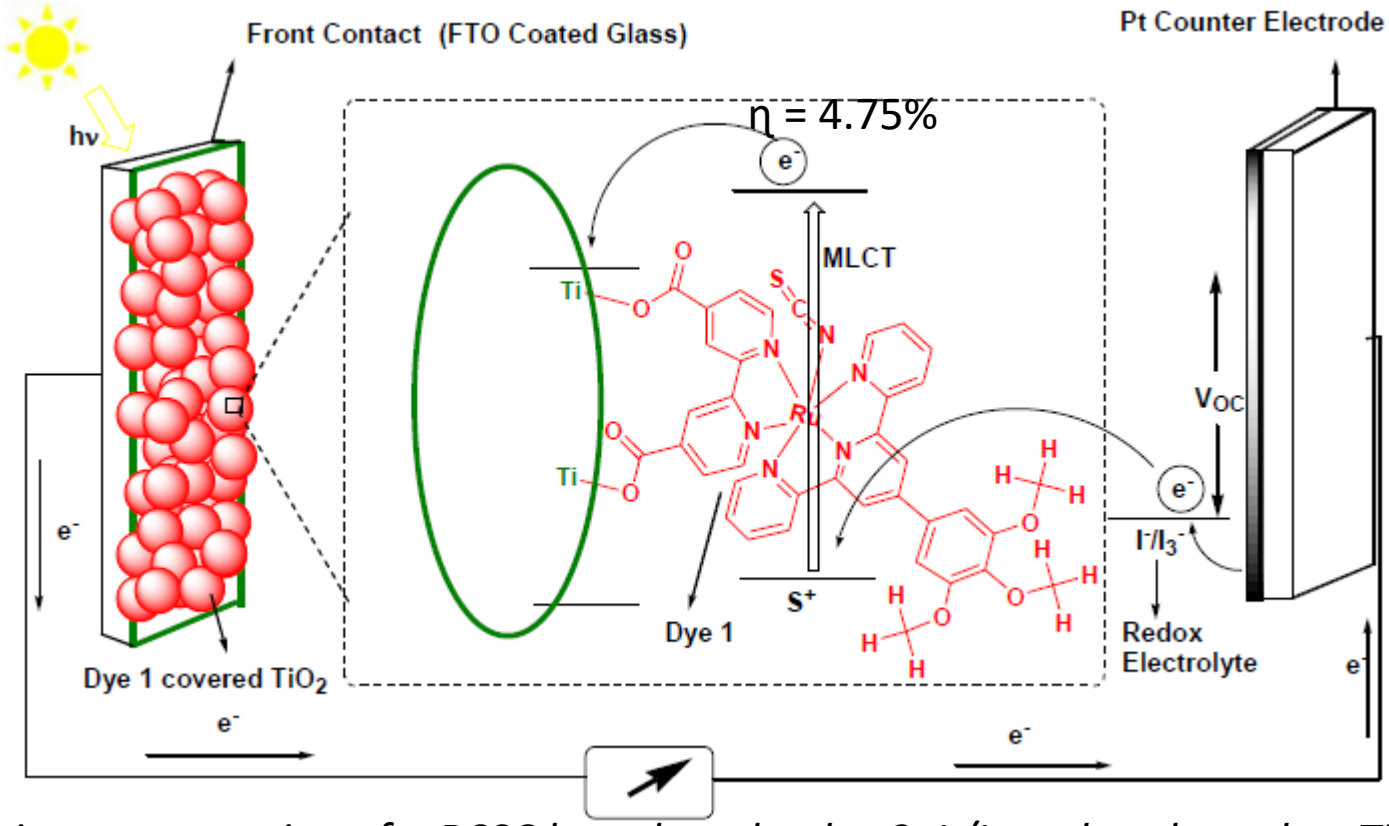
Ongoing PhD student: 1 (regular, self sponsored)

Ongoing work: One Edited book (Nova Publishers, USA)

MoU & Patent: Under planning

Departmental Research Activity

Dye Sensitised Solar Cell (DSSC) Application of Ruthenium based Dyes



Schematic representation of a DSSC based on the dye 3, I^-/I_3^- redox electrolyte,TiO_2 anode and Pt counter cathode

S. Naskar et. al.

Journal of Coordination Chemistry, 2021, doi:10.1080/00958972.2021.1924368

B.N. Mongal et al. / Solar Energy 134 (2016) 107–118

ChemistrySelect 2016, 1, 3276 – 3287

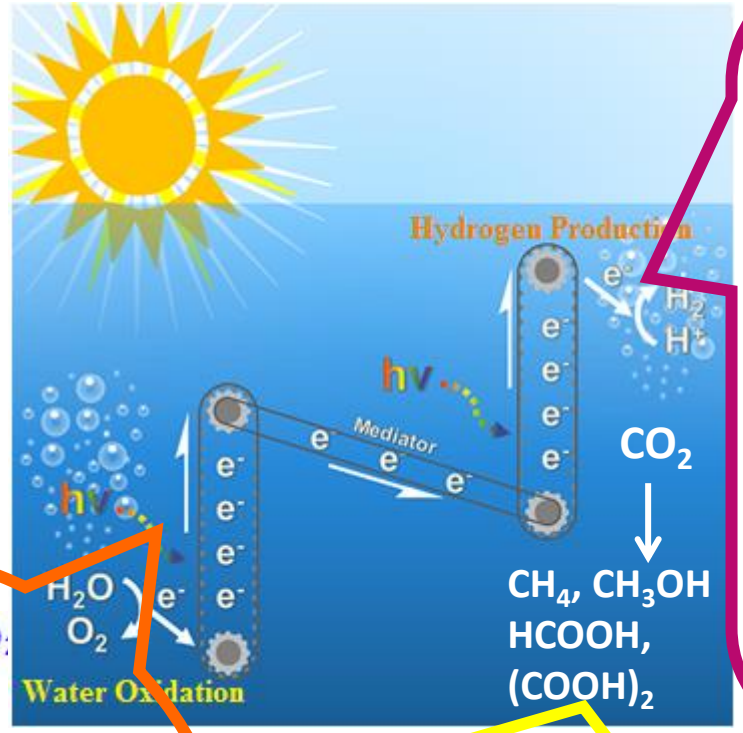
Journal of Coordination Chemistry, 70, 3, 451–462, 2017

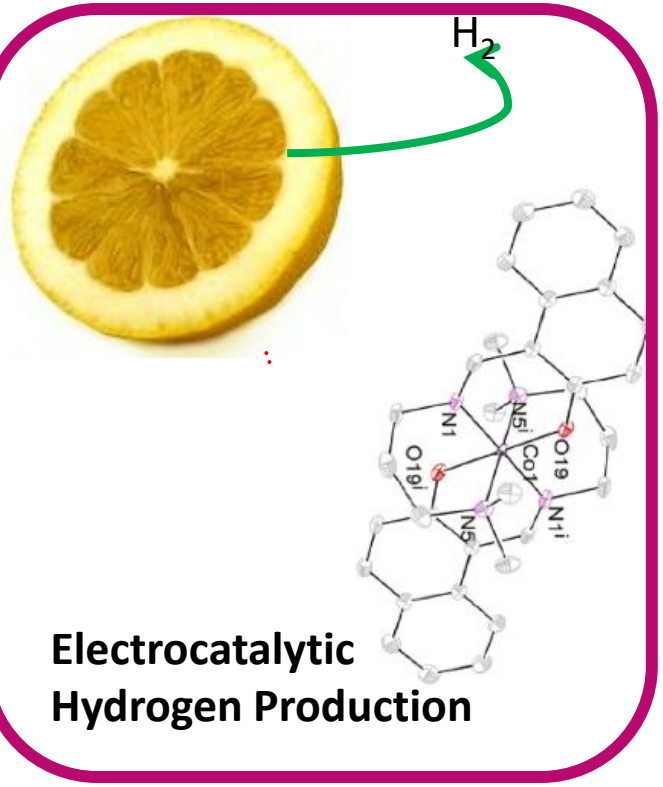
Polyhedron, 102, 615–626, 2015

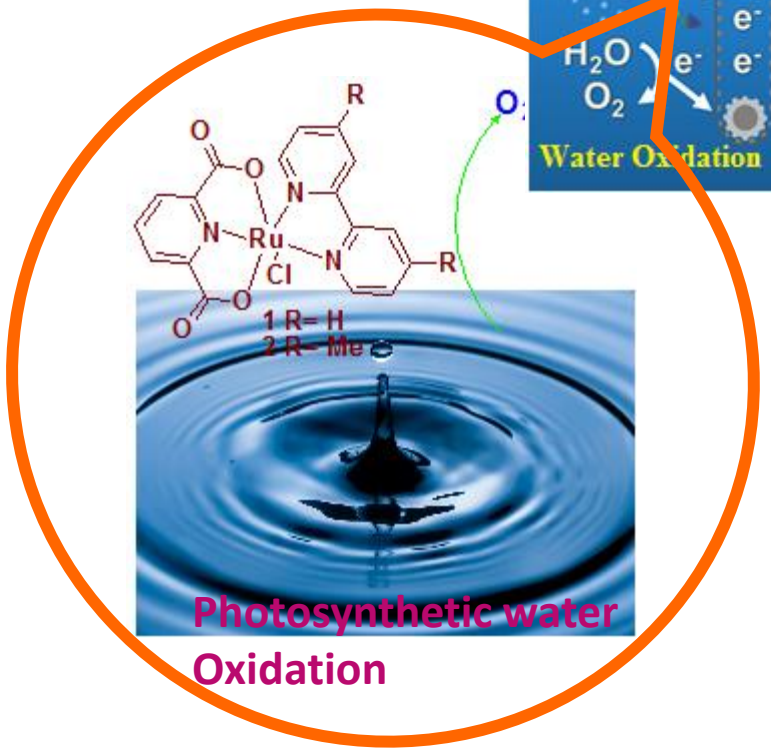
Departmental Research Activity

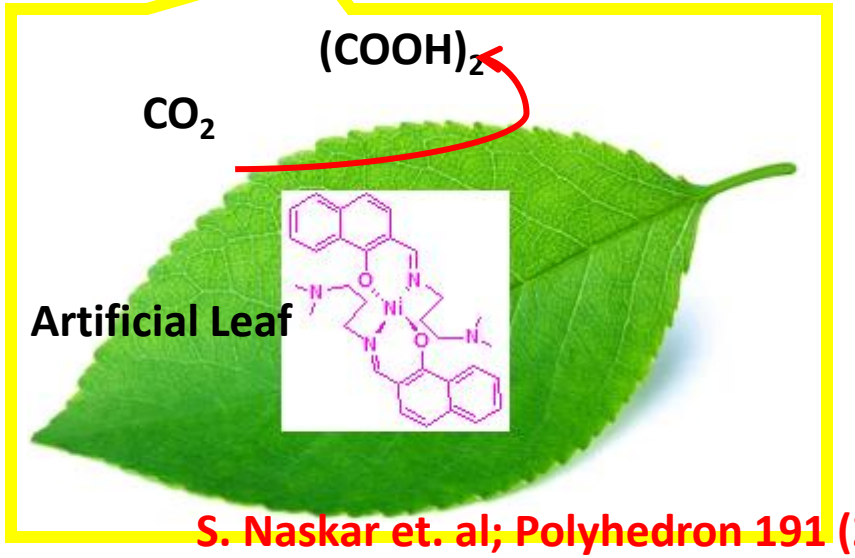
Renewable Energy production by Artificial Photosynthesis

1st Row Transition metal based catalysts







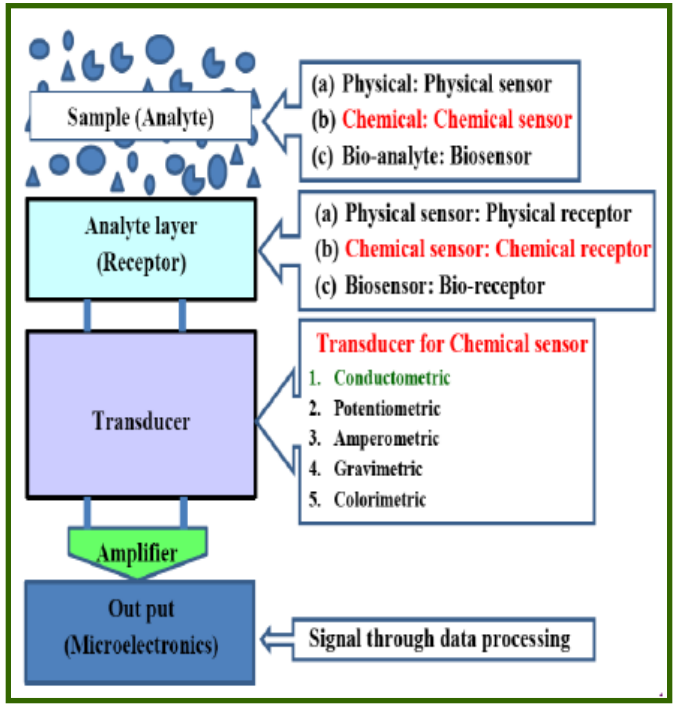


S. Naskar et. al; Polyhedron 191 (2020) 114798

Departmental Research Activity

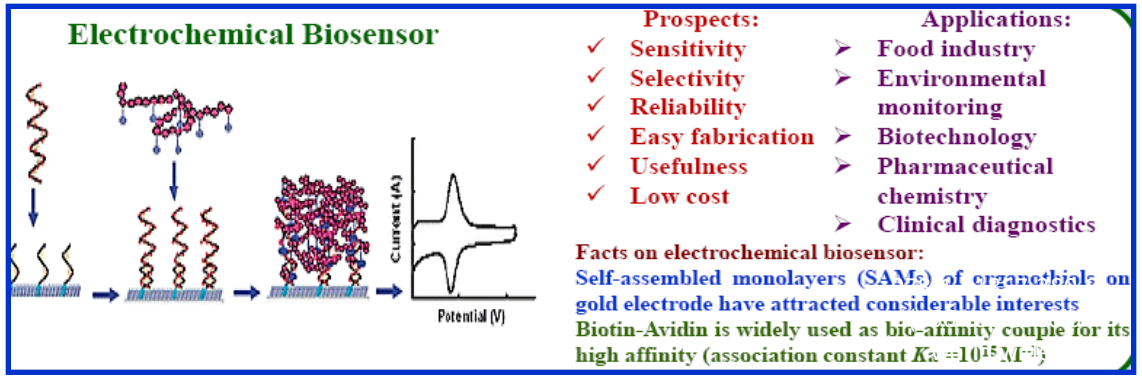
Research Topic: Chemical and Bio Sensors Based on Functional Conjugated Polymers and Nano-materials

Sensors: Measures a physical quantity and converts it into a signal which can be read by an observer or by an instrument. VOCs sensors are useful (especially alcohol sensor) in chemical/food industry, clinic, agriculture filed etc. Selectivity is a real problem.



Receptor: Functionalized conjugated polymers or its nanocomposites

- The functional conjugated polymers (polyaminophenol, polyphenylenediamine) posses processibility, moderate conductivity and better interaction with analyte.
- The inorganic nanomaterials (Cu, funct. CNT etc.) posses good conducting and electro catalytic properties to enhance conductivity, sensing performance, as well as selectivity.



Departmental Research Activity

Research Topic: Chemical and Bio Sensors Based on Functional Conjugated Polymers and Nano-materials

Significant innovation in research

1. Novel route for synthesis of processable active functionalized ICP (e.g., Polyaminophenol, polyphenylenediamine) & nanocomposite
2. New stable doping of those polymers & nanocomposites
3. Sensor set-up design and successful sensing of VOCs (Alcohols)
4. Modification of Au electrode by functional nano-Ag for bio-sensing

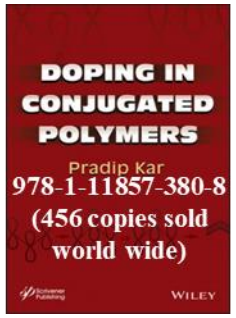
❑ Sponsored Project Completed

1. Preparation of Novel Poly(m-aminophenol)/functionalised carbon nanotube nanocomposites selective sensing for aliphatic alcohol, Sponsored by SERC-DST, Govt. of India, Feb 2012, 3 years (extended to one more year), Rs. 24.95 lakhs, PI: Dr. Arup Choudhury; Co-PI; Working Student: Mr. Sushil Kumar Verma.
2. Induced doping of chemically synthesized processable conducting poly-phenylenediamine, Sponsored by SERB-DST young scientist scheme, Nov 2013, 3 years, Rs. 21.53 lakhs, Sole PI; Working student: Mr. Siddhartha Samanta.
3. Influence of functionalized nanomaterial on electrochemical bio-sensing of biotin-avidin couple; Ref. No. SR/NM/NS-1140/2015; DST Nanomission June, 2016; 3 years, Rs. 40.78 lakhs, Sole PI; Working student: Mr. Nirgaman Bage.

- ❑ Paper Publications: 47 (SCI journals)
- ❑ Book Chapter published: 08 (3 sole author)
- ❑ Reference book published: 02
- ❑ Conference Presentation: 16 (in India, Singapore, France)
- ❑ BE Project Completed: 2
- ❑ M.Sc. Project Completed: 5 (Co-PI in 1)
- ❑ Ph.D. Completed: 3 (joint guidance)
- ❑ Ongoing Ph.D. : 3 (sole guidance)

❑ Significant journal publication (as corresponding author)

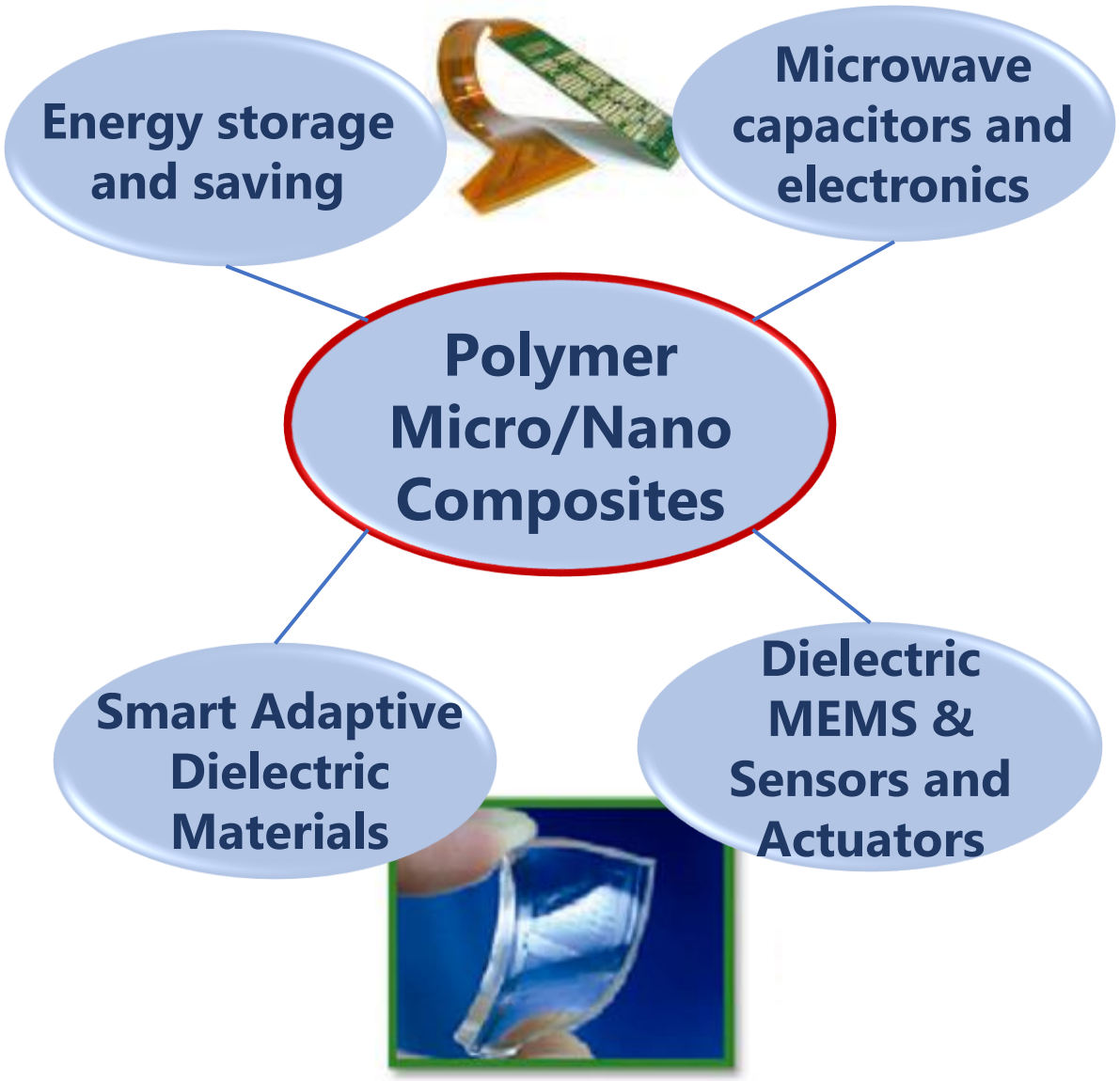
1. S. Kumari, A. Shruti, N. Bage, B.D. Ghosh, P. Kar, J. Env. Chem. Eng. 8 (2020) 104536. IF 4.3
2. S. Samanta, P. Roy, P. Kar, IEEE Sensors J. 20 (2020) 8973. IF 3.073
3. S. Samanta, P. Roy, P. Kar, Mater. Sci. Eng. B 256 (2020) 114541. IF 4.706
4. A. Singh, S. Samanta, N. Bage, B.D. Ghosh, P. Kar, P. Roy, Fun. Mat. Lett. 12 (2019) 1950076. IF 2.00
5. M. Bhuyan, S. Samanta, P. Kar, Elec. Mater. Lett. 14 (2018) 161. IF 1.894
6. S. Samanta, P. Roy, P. Kar, Polym. Adv. Technol. 28 (2017) 797. IF 2.10
7. S.K. Verma, A. Choudhury, P. Kar, Chem. Sel. 2 (2017) 3917. IF 1.811
8. S. Samanta, P. Roy, P. Kar, Macromol. Res. 24 (2016) 342. IF 2.047
9. S.K. Verma, A. Choudhury, P. Kar, Physica Status Solidi A 212 (2015) 2044. IF 1.606
10. P. Kar, F. Tatard, G. Lamblin, P. Banet, P.H. Aubert, C. Plesse, C. Chevrot,l. J. Electroanal. Chem. 692 (2013) 17. IF 3.190



Departmental Research Activity

Synthesis and applications of polymer matrix composites (PMCs)

- Committed to the development of engineering composite materials using contemporary technologies.
- Synthesis of *ceramic* and *metal oxide* nanoparticles *via* chemical solution route.
- Fabrication of metal oxide and/or ceramic *reinforced* polymer matrix composites by *solution casting* and hot-press methods.
- The applications investigated for the synthesized composite materials are as follows:
- PMCs could be further used in Environmental, Biochemical applications



Departmental Research Activity

Dr. Deep Shikha (M.Sc., Ph.D), Assist.*Professor*

Area of Research: Synthesis of New Biomaterial, Surface Modification of Biomaterials

R & D Projects:

Completed (As PI): 17.5 Lac

Ph.D. Supervision:

Awarded :1	Pursuing : 1

PG Supervision:

M.Sc. :6		Pursuing : 1

Publications:

Research Paper	Book
Total Publications in Journal : 11	**Ion implantation in alumina for improved biocompatibility** **Publisher:** LAP Lambert Academic Publishing (18 January 2012)
Papers in Conference : 02	
Conference Attended: 02	

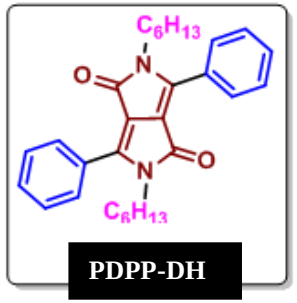
Award & Recognition: **Citations : 44, h-index: 4, i-10 index: 2**

DST-SERC Fast Track Young Scientists Award, 23rd August 2010

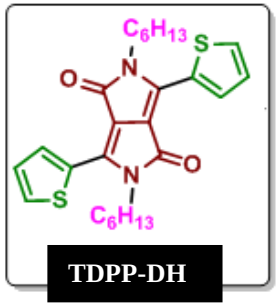
New Dimension: Departmental Research Activity

Earlier Research work on Organic Semiconductors for FET Application

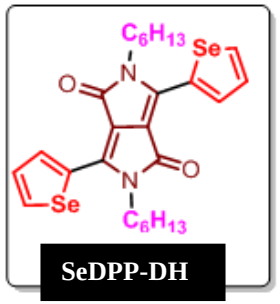
- *Advantageous due to mechanical flexibility, lightweight, low-temperature processing, low cost*



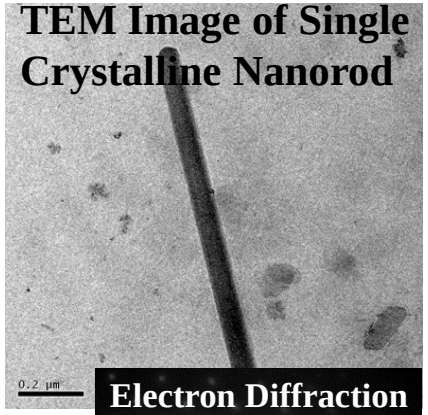
PDPP-DH

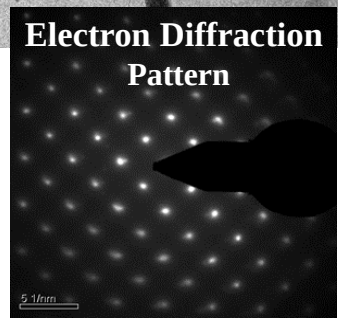


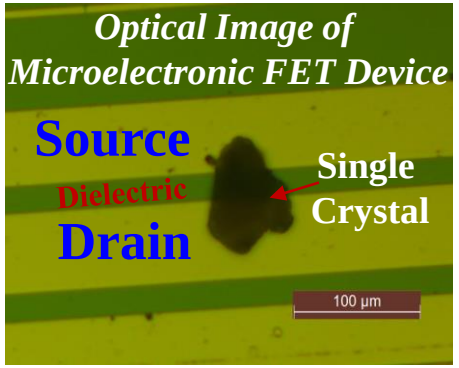
TDPP-DH



SeDPP-DH

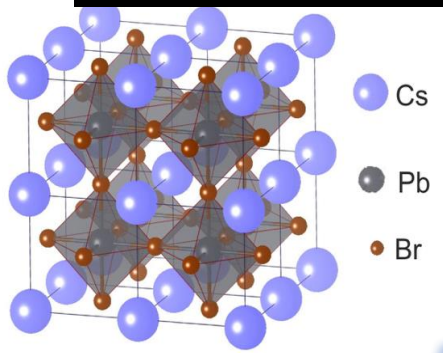


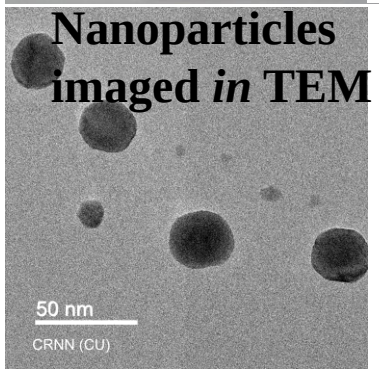


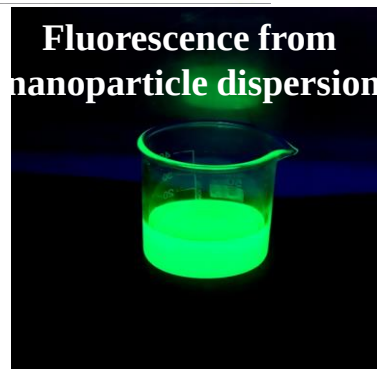


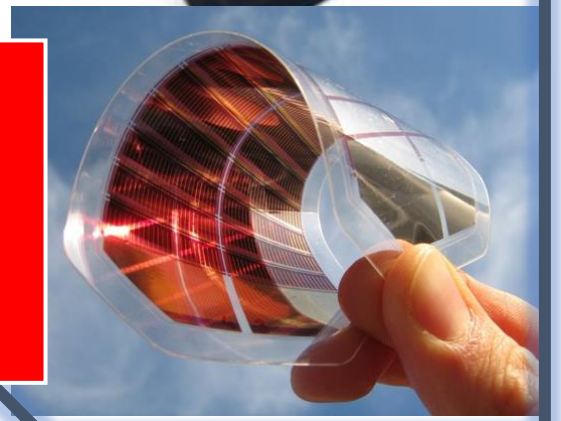
Present Research work on Inorganic Semiconductors for LED Application

- *Advantageous due to easier synthesis, robustness, longer stability*









Future Research Plan on Organic-Inorganic Hybrid Semiconductors for Electronic Applications, viz. Solar Cell, LED, FET, Photodiode

New Dimension: Departmental Research Activity

List of Selected Publications

1. NMR Study of Defect Induced Magnetism in Methylammonium Lead Iodide Perovskite, ***Phys. Rev. B*** 2020, 101, 094417.
2. Lattice Defect Induced Piezo-Response in Methylammonium Lead Iodide Perovskite Based Nanogenerator. ***ChemistrySelect*** 2018, 3, 5304-5312
3. Positron Annihilation Spectroscopic Investigation on the Origin of Temperature-Dependent Electrical Response in Methylammonium Lead Iodide Perovskite, ***J. Phys. Chem. Lett.*** 2017, *8*, 1745–1751
4. Trends in Molecular Design Strategies for Ambient Stable n-Channel Organic Field Effect Transistors, ***J. Mater. Chem. C*** 2017, 5, 7404–7430
5. Herringbone to Cofacial Solid State Packing *via* H-bonding in Diketopyrrolopyrrole (DPP) Based Molecular Crystals: Influence on Charge Transport, ***Chem. Commun.*** 2015, *51*, 97-100

Ongoing Project

AICTE-TEQIP CRS research grant of **Rs. 11.45 lakh** for the project titled "**Band-Gap Engineering of Lead-Free Perovskite Quantum-Dots for Optoelectronic Application**" in the year 2019-2021.

Future Projects

1. Development of n-type polymers for perovskite solar cell to synergistically improve performance and device stability.
2. Organic ferroelectric polymer modulation to improve energy conversion efficiency and stability of perovskite solar cell.
3. Improving electrochemical stability-window of organic-inorganic halide perovskite by structural modification.

Scope of Facility Development

- ❑ **Nanomaterial and Semiconductor Characterization Lab**
- ❑ **Electronic Device Fabrication and Characterization Lab**

Instruments

- ✓ Glove-box, Thermal Evaporator, Solar Simulator with EQE measurement, Optical Profiler
- ✓ FESEM, TEM, AFM, Probe-station

Participating Departments

- ❑ **Chemistry**
- ❑ **Physics**
- ❑ **Electronics and Communication Engineering**

Institute for Collaborative Research Work

- ❑ **IISc. Bangalore, Variable Energy Cyclotron Centre (VECC), NIT Meghalaya, IIT Hyderabad, Jadavpur University**

Thank You