

DEPARTMENT OF CHEMISTRY

(DST FIST SUPPORTED)



NEWSLETTER

ChemOreiká
JULY-DECEMBER'23

BIT MESRA, RANCHI

EDITORS

DR. SUMIT MISHRA
DR. JOYDEEP DHAR



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Message from the Vice Chancellor

Prof. Indranil Manna,

JC Bose Fellow

FTWAS, FNA, FNAE, FNASc, FASc, MAPAM, FIE(I),

FIIM, FEMSI, FAScT, PRS, DSc (hc), PhD

[President, Indian National Academy of Engineering]



BIRLA INSTITUTE OF TECHNOLOGY

MESRA - 835215, RANCHI (JHARKHAND), INDIA

Prof Indranil Manna

Vice-Chancellor

प्रो. इन्द्रनील मन्ना

कुलपति



बिरला प्रौद्योगिकी संस्थान

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12th March 2024

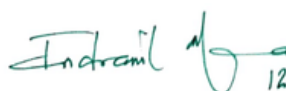
MESSAGE

I am pleased to know that the Department of Chemistry has decided to publish a Departmental Newsletter. I hope this Newsletter will serve as an effective platform to disseminate relevant information about the progress in academic, research and related matters at regular intervals to the concerned community covering faculty and staff members, students and scholars, entrepreneurs, recruiters, industry and alumni. It should also provide a stimulus to encourage the Department to network with partner Departments in all major academic and research organizations and industries.

The Chemistry Department of BIT Mesra is one of the oldest and most reputed Departments in the Institute. The Department is always enthusiastic about conducting various courses and workshops for the faculty and students and training programs for research and scientific advancements.

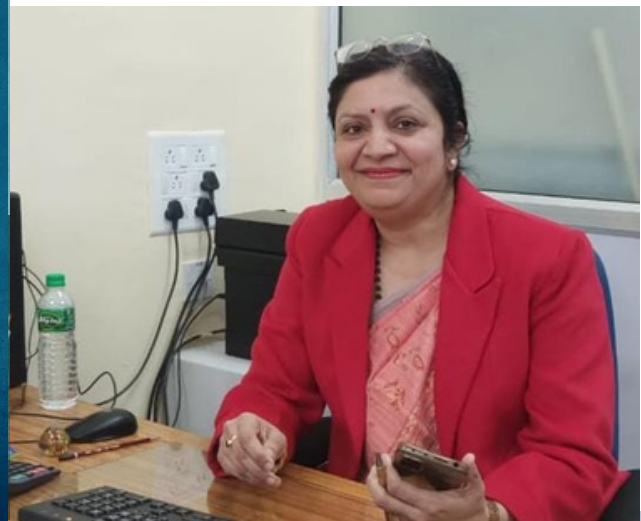
I wish to extend my best compliments to the team constituted for publishing the Newsletter. I sincerely hope this noble initiative will promote and boost the culture and spirit of excellence in academic pursuit in the Chemistry Department and synergise with the rest of the Institute.

Best wishes!


12.03.2024
(Indranil Manna)

From the Desk of HOD

**DR. SUMIT MISHRA,
ASSOCIATE PROFESSOR
HOD, DEPARTMENT OF
CHEMISTRY**



It gives me immense pleasure to give an overview of our Department through the very first edition of this newsletter 'ChemOreiká' which shall serve as an interface between the departmental activities and its various stakeholders.

The department has been an integral part of the institute since its inception in 1955 and is committed to providing quality education in pure and applied chemistry across various domains. We have witnessed continuous growth and development in terms of sponsored projects, publications, patents, advanced research facilities, national and international collaborations, technology transfer, and many more. Our graduated students who have made us immensely proud through their achievements, are our brand ambassadors across the globe.

Our state-of-the-art laboratories serve as a backbone for our commitment to advanced research facilities in specialized areas which are at par with global standards. The department plans to expand its horizons in terms of education and research, outreach activities, training programs, conferences, seminars and workshops and other activities for the holistic development of our students and a vibrant work environment.

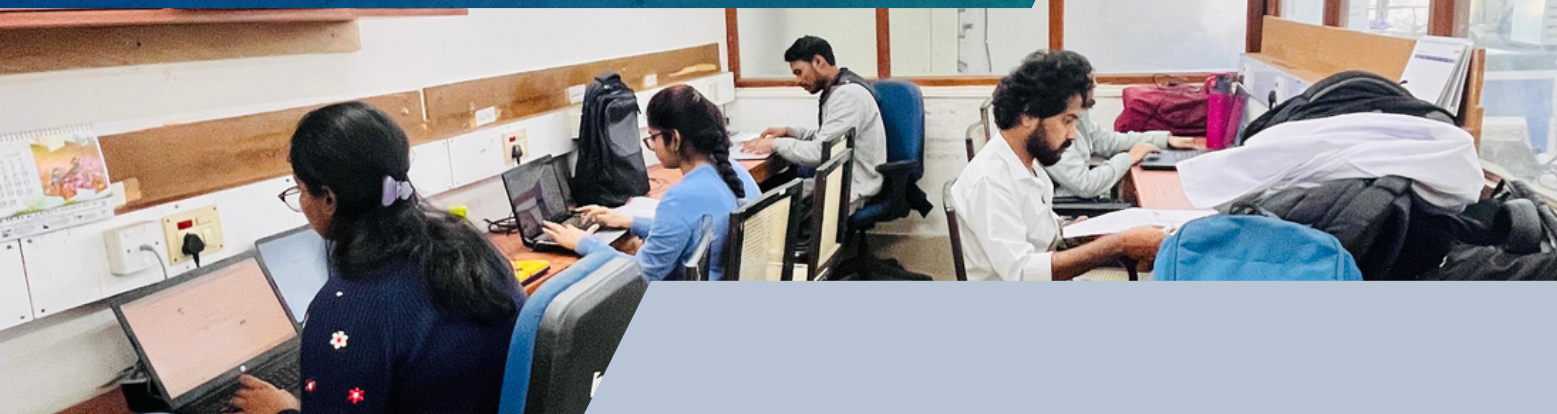
The July to Dec'23 period had a total of 9 sponsored ongoing projects worth Rs. 2 crore 47 lakhs (approx.), 23 publications, 4 patents were filed, and some more are underway.

With these words, I express gratitude to all the people associated with us and look forward for continuous support to explore new horizons for advanced research, and scientific development contributing to a holistic society.

DEPARTMENT OF CHEMISTRY,
BIT MESRA



COURSES OFFERED



Ph.D



M.Sc.



B.Sc. /Integrated M.Sc.

The Department of Chemistry offers Doctor of Philosophy (PhD) after postgraduation/masters in the related subject. At present, more than 30 PhD scholars are enrolled in the PhD programme through CSIR(NET), UGC, SERB (DST), Institute Research Scheme and self-sponsored modes.

2-Year MSc. Chemistry and 5-Year Integrated MSc. (IMSc.) Chemistry based on CBCS guidelines are the ongoing programmes.

4-Year BSc. Chemistry (Honors) or BSc. Chemistry (Honors with Research) followed by 1 Year MSc. Chemistry Research programme has been introduced from the Monsoon 2023 as per the guidelines of the recent National Education Policy (NEP2020).

The multiple entry-exit options are available after successful completion of each year enabling flexibility and continuity in education.

Following certifications shall be awarded based on the duration of the course attended:

- 1-Year Programme: Certificate Chemistry
- 2-Year Programme: Diploma Chemistry
- 3-Year Programme: B.Sc. Chemistry (Major)
- 4-Year Programme: B.Sc. Chemistry (Honors) or B.Sc. Chemistry (Honors with Research)
- 5-Year Programme: MSc. Chemistry Research

Lateral entry at each level is available in the Monsoon session, around July-August each year

Faculty Profile

The department is engaged in pure chemistry, applied and interdisciplinary research in all branches of chemistry, specializing in emerging materials for various applications from biomaterials, environmental remediation, energy harvesting materials, composites, sensors, supercapacitors, drug discovery and molecular modelling to theoretical chemistry and quantum chemistry research.

SPECIALIZATION IN CHEMISTRY

INORGANIC



Dr. Sumit Mishra



Dr. Subhendu Naskar



Dr. Barnali Dasgupta Ghosh



Dr. Deep Shikha



Dr. Atul Kumar

RESEARCH AREAS:
Biopolymers & Biomaterials,
Coordination Chemistry,
Bioinorganic Chemistry,
Nanomaterials &
Nanocomposites,
Supramolecular Chemistry.

PHYSICAL



Prof. P. K. Chattaraj



Prof. P. K. Srivastava



Dr. S. S. Mahapatra



Prof. J. P. Pandey



Dr. Gautam Sen



Dr. Joydeep Dhar



Dr. Debdutta Chakraborty

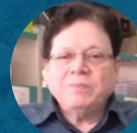
RESEARCH AREAS:
Computational Chemistry,
Electrochemistry, Polymers,
Energy Materials.

RESEARCH AREAS:
Medicinal
Chemistry, Molecular
Modeling and Drug Design,
Sensor Materials, Materials
for Energy Storage

ORGANIC



Prof. Ashoke Sharon



Prof. Amit Basak



Dr. Pradip Kar



Dr. Chandralata Bal



Dr. Anirban Pradhan

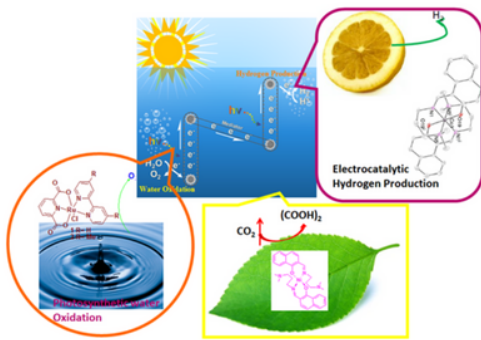


Dr. Bimal Verma

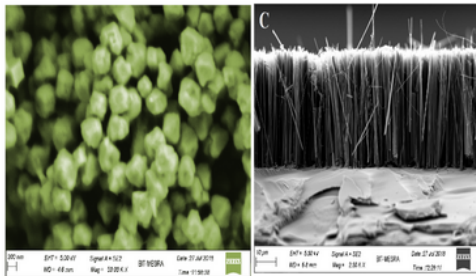
Energy & Advanced Materials

We work on harvesting clean energy and alternating energy resources like solar, piezo and fuel cells. Research groups of Dr. Subhendu Naskar, Dr. Susanta Sinha Mahapatra, Dr. Barnali Dasgupta Ghosh, Dr. Anirban Pradhan, Dr. Pradip Kar, Dr. Atul Kumar and Dr. Joydeep Dhar are pursuing research on the following domains.

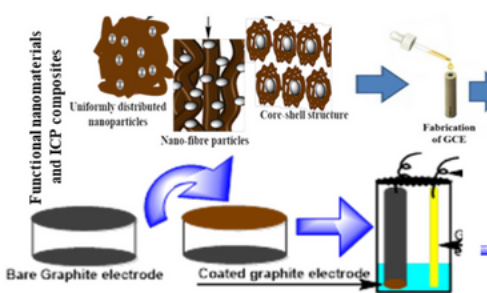
RESEARCH HIGHLIGHTS



Artificial Photosynthesis
(S. Naskar et al.)

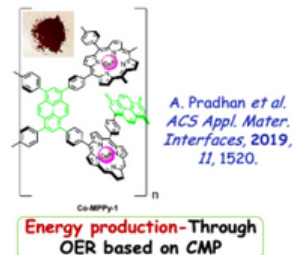
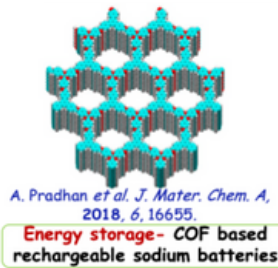


Electrochemical Supercapacitor Applications
(S. S. Mahapatra et al.)

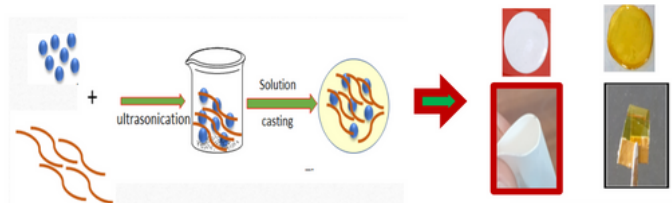


Chemical and Bio-Sensor Applications
(P. Kar et al.)

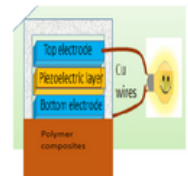
Design and Synthesis of Functional Molecular Architectures
(A. Kumar et al.)



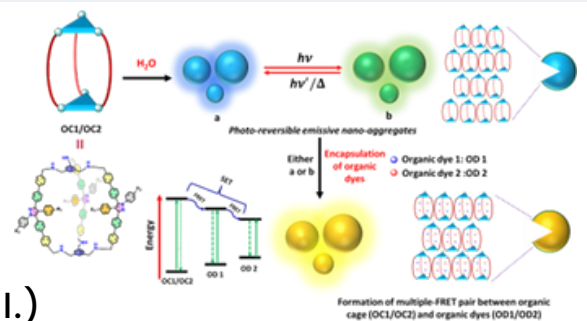
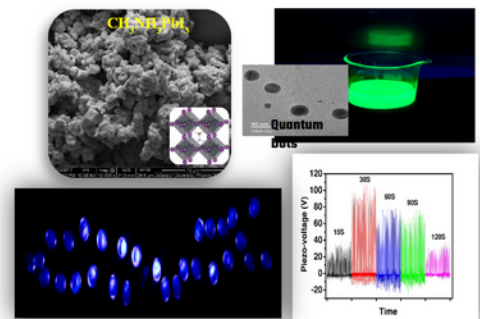
Hydrogen production through water-splitting
(A. Pradhan et al.)



High Dielectric and Energy Storage Applications
(B. Dasgupta Ghosh et al.)



Piezovoltaic and Optoelectronic Applications
(J. Dhar et al.)



Biomaterials & Environmental Research

We are working on modification of biomaterials, polymers, metal organic frameworks, hybrid materials, adhesives and other emerging materials for various applications. The research groups of Dr Sumit Mishra, Dr Deepshikha, Dr Gautam Sen and Dr JP Pandey are pursuing research in these areas.

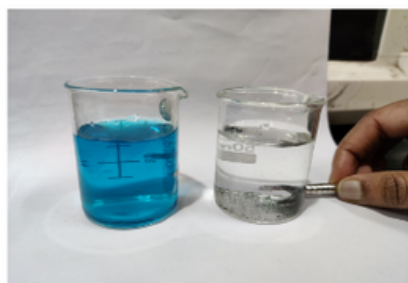
RESEARCH OBJECTIVE

Sustainable solutions to water remediation

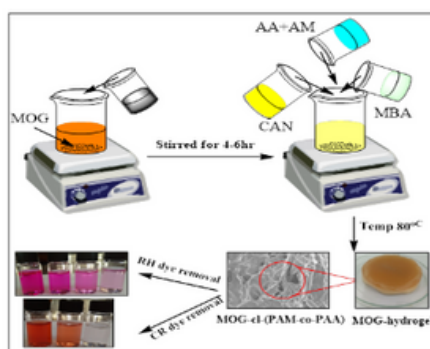
Synthesis process of Biobased materials

Drug, nutrient release matrices, adhesives

Biocompatible materials & applications

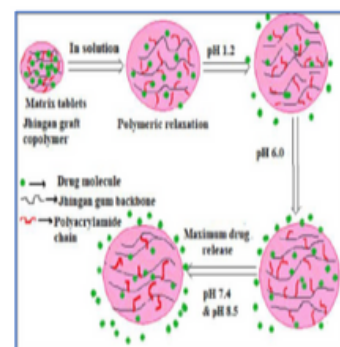


Magnetic Hydrogels for Dye Removal
(S. Mishra et al.)

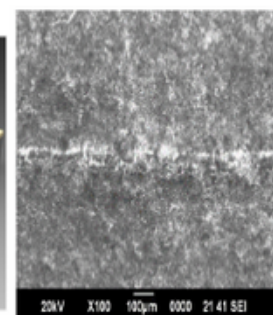
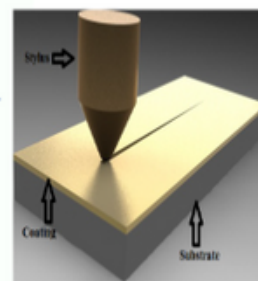
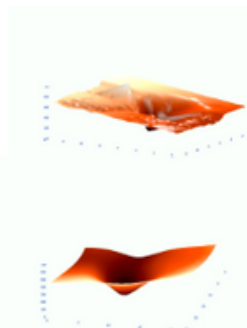


Synthesis of Hydrogels for Water Purification
(S. Mishra et al.)

RESEARCH HIGHLIGHTS



Polymeric Matrix for Drug Release
(G. Sen, J. P. Pandey et al.)



Ion implantation and Adhesion Studies
(DeepShikha et al.)

MAJOR OUTPUTS TILL NOW:

Research grants: 1.61 Cr

- Dr Sumit Mishra developed polymeric materials with 97% efficiency in water treatment; 85% drug & nutrient release, adhesive materials
- Dr Deepshikha developed biomaterials for hard tissue implants
- Dr Gautam Sen & Dr JP Pandey developed Dadmac based materials, fruit juice clarification and flocculants

Awards & Achievements:

- SERB SIRE Award BIT Mesra & SRUC, UK.
- DST STUTI Award under IIT ISM
- DST Young Scientist grant (2)
- Women Scientist Scheme grant
- Young Scientist Award
- CSIR SRF
- PhD thesis Award with cash prize 2000 USD

MAJOR SCIENTIFIC OUTCOME

Technology Development in future:

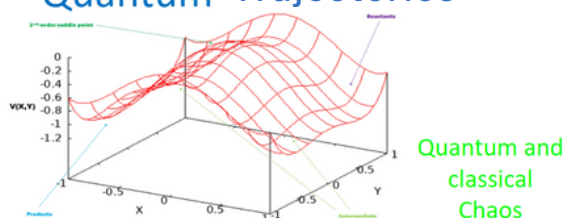
- Water treatment system for onsite treatment
- Multifunctional adhesive hydrogels
- Matrices for drug and nutrient release
- Biomaterials for heart tissue implants



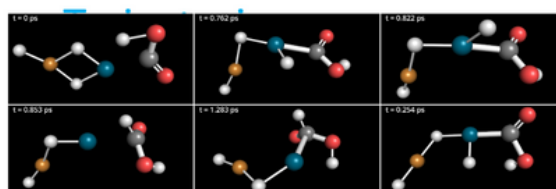
Computational Chemistry and Drug Designing

The Department of chemistry is involved in research on computational chemistry in the field of medicinal chemistry, homogeneous catalysis, optical and magnetic properties of materials/molecules, impact of confinement on reactivity using quantum, classical and quasi-classical methods. In addition to the applied aspects, we also seek to understand fundamental aspects of theoretical chemistry in the domain of conceptual density functional theory (CDFT) and quantum dynamics (Quantum-classical correspondence, control of reaction dynamics, impact of higher order saddle points on reaction dynamics etc.). Dr. P. K. Chattaraj, Dr. D. Chakraborty, Dr. A. Sharon, Dr. C. Bal, Dr. S. Naskar, Dr. J. Dhar, Dr. A. Pradhan and Dr. A. Kumar are pursuing research on these aspects.

Quantum Trajectories

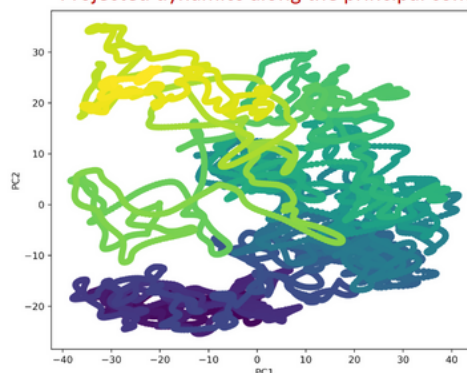


Quasi-classical



HCOOH production from metal Hydride cluster

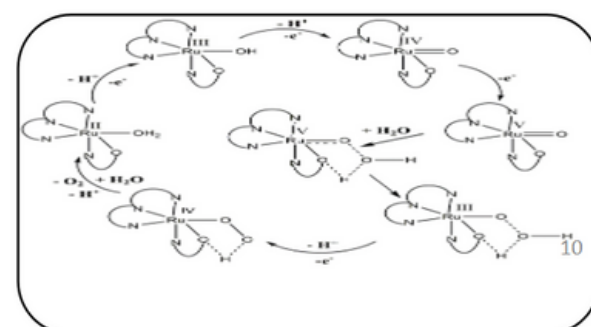
Projected dynamics along the principal components



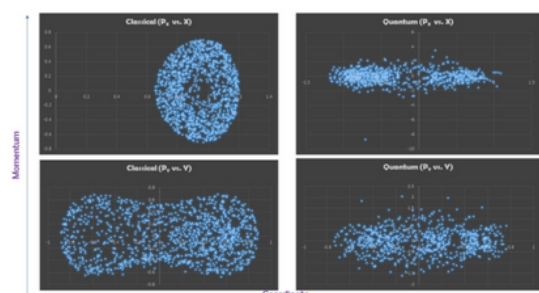
Facilities Available

High end work stations (GPU enabled)

Commercial Software Packages such as Gaussian 16, Schrodinger Suite 2014

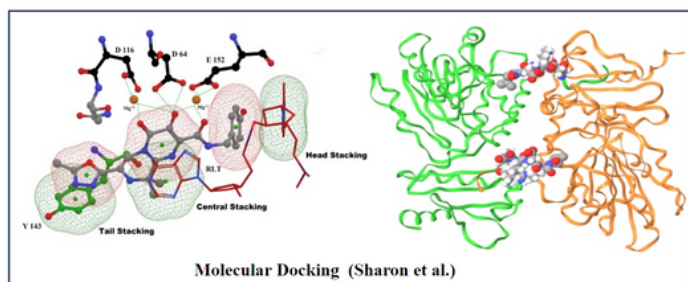


Mechanism of water oxidation through DFT calculation (S. Naskar et al.)

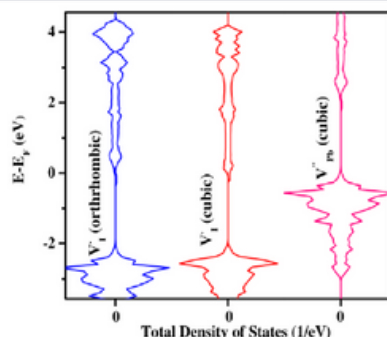


Quantum equivalence of classical Chaos has been explored herein (Chakraborty et al.)

The atomistic reaction mechanism and concerned kinetics in CO₂ hydrogenation reaction is being explored herein (D. Chakraborty et al.)



Molecular Docking (Sharon et al.)



Theoretical analysis of defect-mediated magnetism in lead halide perovskite (J. Dhar et al.)

DEPARTMENTAL ACTIVITIES

Prof. T. K. Paine from IACS, Kolkata, Prof. Suman Chakraborty, IIT Kharagpur, Prof. Vinod Tiwari, IIT BHU visited the Department of Chemistry and delivered lectures on the field of their expertise. These interactive sessions provided new insights to the students, research scholars, and faculty members in their respective research areas.

PROF. VINOD KUMAR TIWARI, BHU

Delivered a Talk on,

“Click Chemistry- A Nobel Prize Reaction:
The Growing Impact on Glycoscience”

18th August, 2023



PROF. T. K. PAINE, IACS KOLKATA

Delivered a Talk on,

“Dioxygen activation by C-C Bond
Cleaving Enzymes: Mechanistic Insights
from Biomimetic Studies”

8th December, 2023

PROF. SUMAN CHAKRABORTY, IIT KHARAGPUR

Delivered a Talk on

“Puzzle and Power of Elementary Chemistry:
How it Can Touch Human Lives”

16th December, 2023



DEPARTMENTAL ACTIVITIES



FAREWELL PROGRAM OF DR. USHA JHA 18TH OCTOBER 2023

After an illustrious career of three decades at BIT Mesra, Prof. Usha Jha retired on 18th October 2023. The Department of Chemistry bid her farewell with good wishes for a happy and healthy life ahead.

ONE-DAY CHEMISTRY OUTREACH PROGRAM KAIRALI SCHOOL: 10TH NOVEMBER 2023

The department conducted a school outreach program in which 300 students from Kairali School, Ranchi participated with their teachers. The students were very enthusiastic to learn about new advancements in science and technology, they visited various facilities of the institute, and a counselling session was also conducted by our faculty to address their queries.



ONE-DAY INTER-SCHOOL CHEMISTRY QUIZ CONTEST-2023; CHAMPION JVM Shyamali 16TH DECEMBER 2023

An interschool chemistry quiz was organized with an overwhelming response of participation from 20 schools with their teams. The students had a tough and interesting quiz competition in various categories which was rejoiced by the audience, It was a real delight for the students to have interactive sessions with our subject experts. On this occasion, Prof. Suman Chakraborty from IIT Kharagpur delivered the inaugural lecture to motivate students for their future in science.



ACHIEVEMENTS

The Department of Chemistry is supported by SERB, DST, DBT, BRNS, CSIR, AICTE, UGC and other extramural funding agencies. The institute supports us in terms of new facilities, seed money grants and all other possible avenues, as and when required.

Currently several projects from SERB, DBT and DST are under implementation amounting approx. Rs 2 crore 47 lakh. In last six months 23 research articles were published in peer-reviewed internationally acclaimed journals with the highest impact factor of 15.1 by Dr. Barnali Dasgupta Ghosh.

- ★ Professor Pratim K. Chattaraj received a special honor from Theoretical Chemistry Accounts journal which published a special Festschrift issue on his sixty-fifth birthday to commemorate his research contributions to Theoretical and Computational Chemistry in general and Density Functional Theory in particular.
<https://link.springer.com/collections/cfdiieejfc>
An international conference was also organized to commemorate this occasion.
- ★ He was also selected among highly cited researchers worldwide (top 2 % bracket) according to Standford/Elsevier Data Repository. He was the recipient of Chemistry in India Leader Award (2023). He delivered Professor Prafulla Chandra Ray Memorial Lecture Award (NASI).
- ★ Dr. Debdutta Chakraborty received certificate of appreciation for publishing research in the top 10% of highly cited works from the Royal Society of Chemistry, UK Journals.
- ★ Dr. Joydeep Dhar has received Start-up Research Grant (SRG) of Rs. 30 Lakh from SERB.
- ★ Four Patents by Dr. Sumit Mishra, Dr. Gautam Sen, Dr. Deep Shikha and Dr. Anirban Pradhan were published and some more were applied.
- ★ PhD scholar Leena Priya, from Dr. Pradip's Kar lab received Best Poster Presentation Award from ACS in the International Conference on Integrative Chemical Science for Health & Environment-2023 (ICHE 2023) held at the Deshbandhu College, Department of Chemistry, University of Delhi, on 06-08 October 2023.



Nisha Kumari from Dr. Sumit Mishra's lab received her PhD degree on 1st October 2023.

Sahanwaz Khan from Dr. Subhendu Naskar's lab successfully defended his thesis on 8th December 2023



Message from Alumni



Name: Dr. Ch. Jamkhokai Mate
PhD: BIT Mesra
Designation: Scientist
Organization: Indian Council of Agricultural Research (ICAR)-Indian Agricultural Research Institute (IARI), Assam, Govt. of India
Mobile No: 7366092535 **E-mail:** kakaiiari@gmail.com

It gives me immense pleasure to recapitulate the excellent career I have pursued under the dynamic guidance of my PhD Supervisor, Dr. Sumit Mishra, the Present HOD, Department of Chemistry, BIT Mesra. My Ph.D programme was in accordance with my organization mandate and the topic of my Ph.D work was ‘Synthesis and characterization of modified Jhingan gum derivatives and their applications’. The experience I have in my Ph.D programme plays vital role in my successive works related to my Institute mandate and also it paves the way for other applications particularly in developing farmer need-based products. I have published five research papers within the span of three years which is undoubtedly because of the constant support of my Guide and the amenities available at real-time requirement and not to forget the support of the faculty members in the department. If I have to cite university that gives best quality education, working environment, supporting facilities and other research oriented programme, BIT Mesra hits the first.



Name: Shaini Banerjee
MSc: BIT Mesra
Current Designation: Scientist
Organization: Alexion AstraZeneca Rare Diseases, Ireland
E-mail: shaini.banerjee23@gmail.com

My Masters in Chemistry from BIT Mesra enhances my understanding of the chemical structure and decide the test required to test the raw materials, excipients, API and products while my masters in Biotherapeutics enables me to link the chemistry with the biological activity and study the contamination and how to control it so that everything can be of top quality. Quality is of utmost importance in any pharmaceutical company and especially when working on drugs for immunocompromised kids there is no margin of error. During my masters in Chemistry my project under Prof. Ashoke Sharon “Structural Studies of nucleotide analogues as possible SARS-CoV-2 RdRp inhibitor” enabled me to find my true passion to study more about biologics products and work on them in future. I am a proactive, energetic Quality Control Analyst currently working for Alexion AstraZeneca Rare Diseases in Ireland. As a rare disease unit Alexion deals with complex biological molecules which requires a comprehensive understanding of Chemistry and Biology.

RESEARCH FACILITIES

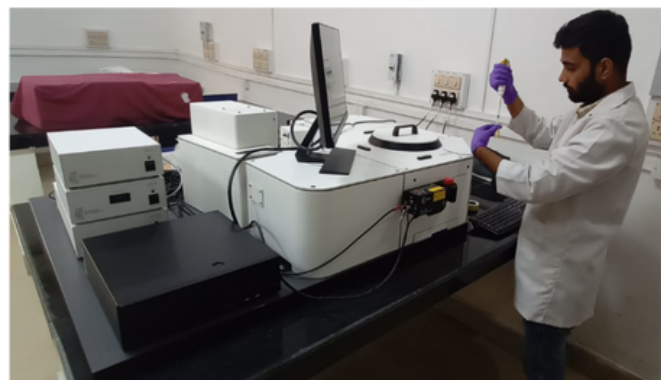
The Department of Chemistry is equipped with several state-of-the-art laboratories with advanced instruments.

The Department houses many sophisticated instruments for in-house and collaborative research

- NMR Spectrometer (400 MHz),
- UV-vis spectrophotometer,
- IR spectrometer,
- Solar simulator,
- Sourcemeeter
- Microwave reactor,
- Rotary evaporator,
- Polarimeter,
- Electrochemical analyzer and others

In last few months new facilities were created.

- A high-end spectrofluorometer FLS1000 from Edinburgh Instruments, UK was installed in the department and after a few days of training and demonstration the instrument is now open for the research scholars to use.
- High performance computing cluster was also installed under the supervision of Dr. Debducta Chakraborty utilizing his Start-Up Research Grant from SERB.
- With the funding from SERB, in last two months two new instruments, namely, electrospinning and lyophilizer were installed in Dr. Barnali Dasgupta Ghosh's lab.



Newly installed FLS1000 Spectrofluorometer from Edinburgh Instruments



High Performance Computing research facility

Lyophilizer from Labfreeze Instruments, China



Electrospinning, Model: ESPIN-Nano by PICO, Chennai

ONGOING PROJECTS

Sl. No.	Project Title	Principle Investigator	Funding Agency	Date of Sanction	Duration of the Project	Sanctioned Amount (Lacs)
1	Combination of small light emitting molecules with carbon materials for next generation optoelectronics	Dr. A. Pradhan	SERB-DST	June,22	3 years	16.0
2	Bottom-up solution phase synthesis of curved polycyclic aromatics, nanographene, carbon nanoribbons and nanobelts for next-generation optoelectronics	Dr. A. Pradhan	SERB-DST	Sep, 22	2 years	31.18
3	Metal organic frameworks and sequential electrocoagulation for remediation of mining effluents	Dr. Sumit Mishra	SERB	March, 22	3 years	25.01
4	Biocompatibility and mechanical studies of nanostructured HAP, metal doped nanostructured HAP on alumina by RF magnetron sputtering	Dr. Deep Shikha	SERB	Feb, 22	3 years	27.72
5	Photo-responsive tetra-aryl pyrazole based emissive organic nano-cage as an artificial-light harvester for heterogeneous photocatalysis	Dr. A. Kumar	DST	Sep, 22	2 years	31.76
6	Direct dynamics simulation study on the catalytic hydrogenation of CO ₂ by some transition metal hydride clusters	Dr. D. Chakraborty	DST	Sep, 22	2 years	23.64
7	Natural product inspired synthesis and biological evaluation of novel pyranone/yyridinone analogs as enhancer of muscle energy expenditure to treat type 2 diabetes	Dr. C. Bal	DST	Sep, 22	3 years	16.17
8	Electrospun PVDF based piezoelectric nanocomposite energy harvesters for self-powered smart wearable and implantable electronics	Dr. B. Dasgupta Ghosh	SERB	Jan, 23	3 years	45
9	Investigating the effect of molecular doping in halide perovskites based energy harvesting devices	Dr Joydeep Dhar	SERB	Dec, 23	2 Years	30.09

RECENT PUBLICATIONS

1. N. Arepalli, S. Mondal, D. Chakraborty, P. K. Chattaraj, Impact of Static Oriented Electric Fields on the Kinetics of Some Representative Suzuki-Miyaura and Metal-Cluster Mediated Reactions Molecules, 2023, 28, 6169.
2. P. K. Chattaraj, R. Pal, A Modified Cusp Condition for the Single Density Equations of DFT and Orbital-Free DFT for Atoms. Journal of Mathematical Chemistry, 2023, 61, 1717–1725.
3. P. Das, R. Saha, P. K. Chattaraj, Metal-Metal Bonds with Unusual Oxidation States in Early s-Block Elements: A Computational Perspective. Polyhedron 2023, 245, 116661. Invited article, Special Issue on, “Chemical Bonding”,
4. R. Jha, S. G. Patra, H. Mondal, P. K. Chattaraj, Theoretical Understanding of Mechanochemical (Ball-Milling) Synthesis of Thioethers: A CDFT Approach. Journal of Mathematical Chemistry 2023, 61, 1825-1841.
5. H. Mondal, P. K. Chattaraj, Unraveling Reactivity Pathways: Dihydrogen Activation and Hydrogenation of Multiple Bonds by Pyramidalized Boron-Based Frustrated Lewis Pairs. ChemistryOpen 2023.
6. T. Chakraborty, P. K. Chattaraj, 2023, Editorial, J. Phys. Org. Chem. Special issue on, 'Density Functional Theory for Exploration of Chemical Reactivity: Successes and Limitations'
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