

About Universities

GMRITDU: Established in 1997, GMR Institute of Technology has grown steadily with a strong focus on academic excellence and ethical values, earning wide recognition for its quality education and consistent performance. In January 2026, it was notified as a Deemed to be University sponsored by GMRIT Foundation (section 8 Company) under Section 3 of the UGC Act, 1956, by the Ministry of Education, Govt. of India. GMRITDU provides its learning community state-of-the-art facilities, infrastructure and a competent faculty. The Institute encourages collaborative learning between industry and academia as a means of reinforcing its curriculum with practical and real-world experiences. All UG programs are accredited by NBA and the institute is accredited by NAAC with 'A' grade. GMRIT University has gained international recognition through its inclusion in THE World University Rankings and THE Impact Rankings across several Sustainable Development Goals (SDGs).

CSIR-IMMT: CSIR-IMMT, Bhubaneswar, was established on 13th April 1964 as the Regional Research Laboratory under CSIR, New Delhi, and was renamed in 2007 to reflect its renewed focus on mineral and materials resource engineering. The institute conducts basic and technology-oriented research addressing critical challenges in the mining, minerals and metals sectors. Its key priorities include advanced and sustainable technologies, zero-waste processing, resource-use efficiency, critical raw materials and advanced materials development. Through multidisciplinary R&D, consultancy, technology transfer, and public-private partnerships, CSIR-IMMT contributes to strengthening Indian industries, enhancing resource efficiency and value addition, promoting innovation, and advancing sustainable development across the mineral and materials value chain.

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Topic: Molecular Modeling and Computational Insights into Bonding, Covalency, and Magnetic Properties of Paramagnetic Transition Metal and Actinide Complexes

Dr. Rambabu Dandela, Institute of Chemical Technology, Bhubaneswar
Topic: Molecules to Medicines: The Role of Quantum Computing in Modern Drug Discovery and Pharmacy

Dr. Chetti Prabhakar, NIT - Kurukshetra
Topic: Computational Investigation of Optoelectronic Properties and Structure-Property Relationships in D- π -A Organic Sensitizers

Dr. Kanakati Arun Kumar, University of Jyväskylä, Finland
Topic: Manipulating Molecules with Mirrors

Dr. Rajagopala Reddy Seelam, Central University of Rajasthan
Topic: Computational Tools for Chemists: GNU Octave and Gaussian Applications in the Study of Triplet-State Generation in BODIPY and Aza-BODIPY Dimers



GMRIT
DEEMED TO BE
UNIVERSITY



GMRIT Deemed to be University

Conducting 5-day Online
Faculty Development Program in
Collaboration with
CSIR - Institute of Minerals and Materials
Technology (IMMT)-Bhubaneswar

Titled
**Computational Methods and Tools
for Applied Physical Sciences:
Fundamentals to Advanced Research**

26th to 30th October 2026

Organized by

Department of Chemistry



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About the Department

Departments of Chemistry, School of Physical Sciences, GMRITDU: The Department of Chemistry, School of Physical Sciences, GMRIT Deemed to be University, is committed to excellence in teaching, research, innovation, and academic advancement. The Department provides a strong foundation in chemistry for students across engineering, science, pharmaceutical, and interdisciplinary programmes. It comprises highly qualified and experienced faculty actively engaged in research across diverse areas of chemistry, including materials chemistry, nanotechnology, environmental chemistry, catalysis, energy materials, and related interdisciplinary fields. Faculty members contribute to quality research publications in reputed national and international journals and actively participate in government-funded research projects. As part of GMRIT Deemed to be University, the Department is strengthening its academic and research ecosystem through national and international collaborations with leading institutions, industries, and researchers. Through quality education, impactful research, innovation, and collaborative initiatives, the Department strives to advance chemical sciences and promote their meaningful applications in academia, industry, healthcare, environment, and society.

About the FDP

Computational Tools and Applications in Interdisciplinary Sciences: From Fundamentals to Advanced Research (CTAIS-2026) is a multidisciplinary Faculty Development Programme focused on modern computational tools and methodologies across Physical, Chemical, Biological, Materials, and Pharmaceutical Sciences. The programme aims to bridge fundamental scientific concepts with computational approaches through modelling, simulation, data analysis, visualization, and research-oriented software.

It provides faculty, researchers, and postgraduate students with expert insights, hands-on training, demonstrations, and practical exposure to computational techniques for scientific problem-solving. The FDP further promotes interdisciplinary collaboration, computational-experimental integration, innovation, and data-driven research, enabling participants to effectively apply emerging computational technologies to contemporary scientific challenges.

Objectives

- Introduce modern computational tools for scientific research and teaching.
- Develop skills in modelling, simulation, data analysis, and visualization.
- Explore computational applications across diverse scientific disciplines.
- Provide hands-on training in programming and computational tools.
- Introduce AI, ML, and advanced scientific modelling techniques.
- Promote interdisciplinary computational-experimental research, innovation, and collaboration.

Topics Covered

- Computational Chemistry and Molecular Modelling
- Gaussian and GNU Octave for Scientific Computing
- Optoelectronic Properties and D- π -A Sensitizers
- Bonding, Covalency and Magnetic Properties of Metal Complexes
- Quantum Computing Applications in Drug Discovery and Organic Synthesis
- Computational Photochemistry and Excited-State Molecular Systems

Contact Persons

Dr. B. Viswanadham : 8985315285

Dr. D. Tejeswara Rao : 9000246424

Eligibility

All interested Faculty, Research Scholars, PG Students, and Industry Personnel.

Registration Details

Faculty, Research Scholars, PG Students : Rs. 300/-

Industry Participants : Rs. 500/-

Bank Account Details for Payment

Account : Indian society of
Technical Education
GMRIT Chapter

Bank Name : Union Bank of India



(Please upload payment receipt copy along with the UTR number while doing registration)

Registration Link

<https://forms.gle/Nth6zV1Fk3DoVaBi8>

