J. C. BOSE UNIVERSITY OF SCIENCE & TECHNOLOGY, YMCA, FARIDABAD

(Established by Haryana State Legislative Act No. 21 of 2009 & Recognized by UGC Act 1956 u/s 22)
Accredited '**A+**' Grade by NAAC

DEPARTMENT OF CHEMISTRY

Organized Seminar on
"AI4Science – From Modelling Chemical Transformations to Understanding Biomolecular Processes"

Name of Department/ Section/ cell conducting the activity	**Department of Chemistry**
Date of conduct	**April 23, 2026**
Activity Coordinator/Convener	**Dr. Anurag Prakash Sunda**
Amount Spent	**Rs. 5500**
Funding/ grant from (University/ Industry/ UGC/ AICTE/ DST/ TEQIP/ Outside Society/ agency/others (mention)	**University**
Target audience	Faculty Members and Students (UG, PG, PhD)
No. of beneficiaries	60+
Outside guests	**Prof. Tarak Karmakar,** Associate Professor, Indian Institute of Technology (IIT) New Delhi
Any other information **Activity Links**	Facebook Link

Flyer

Pics of the event

REPORT SUMMARY

Expert Lecture Explores Expanding Role of AI in Chemical Sciences at J.C. Bose UST, YMCA

Faridabad, April 23 — The Department of Chemistry at J. C. Bose University of Science and Technology, YMCA organized an expert lecture on *"AI4Science – From Modelling Chemical Transformations to Understanding Biomolecular Processes"* on Thursday at the CV Raman Science Block. The event drew active participation from faculty members, research scholars, and students.

The lecture was delivered by **Prof. Tarak Karmakar**, Associate Professor at the Indian Institute of Technology (IIT) Delhi. Prof. Tarak is honoured as Editorial Advisory Board of ACS and Springer Nature Journals. He elaborated on the transformative role of artificial intelligence and machine learning in contemporary chemical research, with particular emphasis on molecular dynamics simulations, enhanced sampling methodologies, and their applications in understanding complex biomolecular systems, advance functional nano materials, and catalysis.

The programme was held under the patronage of **Prof. Rajive Kumar**, Vice-Chancellor of the university, reflecting his commitment to excellence and the promotion of AI-driven research. **Prof. Anuradha Sharma** provided academic guidance and encouraged students to stay abreast of emerging developments in artificial intelligence. The session was chaired by **Dr. Bindu Mangla,** who urged students to harness generative AI tools for addressing real-world challenges. Dr.

Anurag Prakash Sunda served as the convener and coordinated the event. Active participation by scholars and faculty during the question-and-answer session made the programme more engaging and insightful.

The lecture underscored the growing convergence of computational techniques and chemical sciences, offering valuable insights into emerging interdisciplinary research avenues. It concluded with an engaging interactive session followed by a formal vote of thanks. The department also acknowledged **Prof. Ajay Ranga**, Registrar of the university, for his exceptional administrative support in the successful conduct of expert lecture.

Attendees: Around **60 participants** attended the seminar.

Promotion of event on social media: Facebook Link

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