

About IIT Kharagpur



Kharagpur - a beautiful town in the eastern corner of India, famous until 1950 as home to the longest railway platform in the world - became the nursery where the seed of the IIT system was planted in 1951. IIT Kharagpur started its journey in the old Hijli Detention Camp in Eastern India, where some of the country's great freedom fighters toiled and sacrificed their lives for India's independence. Spurred by the success of IIT Kharagpur, four younger IITs sprouted around the country in the two following decades, and from these five came thousands of IITians, the brand ambassadors of modern India. It was the success of this one institution at Kharagpur that wrote India's technological odyssey.

This Institute of Eminence takes pride in its relentless effort to provide the best platform for both education as well as research in the areas of science and technology, infrastructure designs, entrepreneurship, law, management, and medical science and technology. Department of Chemistry of IIT Kharagpur is among the best Chemistry departments of the country with excellent record in teaching and research.



Department of Chemistry, IIT Kharagpur

Program Features/ Structure

Classroom lectures – 50%

Hands-on Computational
Modeling – 50%

Introduction to
Programming and
Molecular Modeling

Program Fee

Nil for TEQIP-III
sponsored participants

For others - INR 6,500/-
(including GST).

This includes
accommodation,
registration, and
working lunch.

Last day of Registration

10

February 2020

Program Schedule and Venue

11 – 13 March 2020 (9:30
AM – 6 PM)

Department of
Chemistry,
IIT Kharagpur

Who will benefit (Eligibility)

Teachers of Engineering
and Science Colleges
interested in teaching
Computational Chemistry
and Physics; Advanced
Post-Graduate Students in
Science and Engineering.

Accommodation

Accommodation will be
provided to the
participants at the
campus Guest house.

How to Apply

Use the link: <https://erp.iitkgp.ac.in/CEP/courses.htm> to
apply ONLINE.



Payment if applicable is to be done **ONLINE** after getting
short listed for the program.

Contact Us

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NPIU

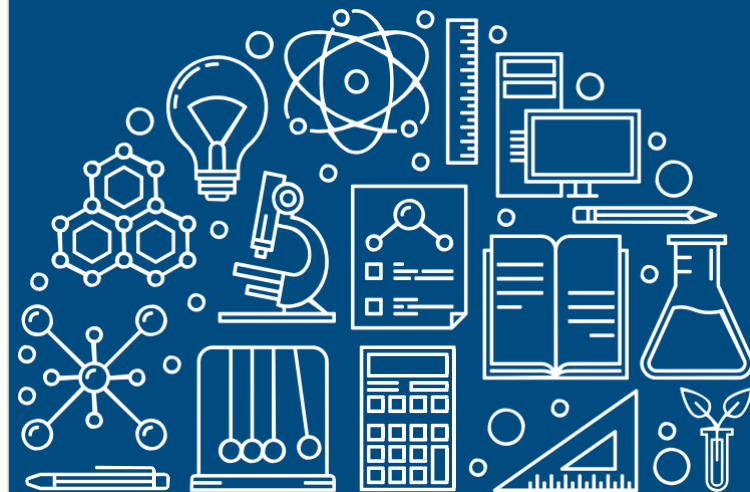
TEQIP-KIT

NPIU - A Unit of MHRD, Govt. of India for
Implementation of World Bank Assisted Projects in Technical Education

Indian Institute of Technology Kharagpur

Applications of Computers in Chemistry

11 – 13 March 2020



Introduction / Overview

Computational modeling has become an integral part of all engineering and science disciplines. With progress in hardware and software, the complexity of the problems that can be modeled is rising. In the recently updated curriculum, UGC has introduced several courses on computational chemistry and physics at the undergraduate level. To stay updated with the modern trends, it is necessary to impart a solid foundation in computational techniques to the post-graduate students as well as the science and engineering teachers involved in undergraduate and post-graduate teaching.

Program Objectives

This course would help the advanced post-graduate students and teachers engaged in teaching science and engineering at undergraduate and post-graduate levels. The course aims to provide a foundation in computational techniques through intensive class room teaching supplemented by hands-on training in programming and molecular modeling.

What you will learn

Program Content

Introduction and Overview of Computational Chemistry

Programming Basics: Constants, variables, operators; evaluating simple math expressions; Data types: lists, strings; Debugging; Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

Introduction to computation and algorithms: Basic algorithms sorting, recursion, brute-force, bisection, iterative procedures, Computational Complexity.

Numerical methods Roots of equations: Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.

Differential calculus: Numerical differentiation. Integral calculus: Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values. Simultaneous equations: Matrix manipulation: addition, multiplication. Gauss-Siedal method.

Handling of experimental data: Interpolation, extrapolation and curve fitting.

Molecular modeling: Potential energy surfaces; Elementary ideas of molecular mechanics and practical MO methods; Simple exercises using molecular visualization software.

About the Faculty

The lectures and laboratory classes will be conducted by experienced and reputed professors from different departments of IIT Kharagpur.

Coordinator

Dr. Anoop Ayyappan
Department of Chemistry



Co-Coordinator

Dr. Sabyashachi Mishra
Department of Chemistry



Other faculty for the course

Prof. P. K. Chattaraj
Department of Chemistry



Dr. Parag Deshpande
Dept. Chemical Engineering



Dr. Divya Nayar
Centre for Computational
and Data Science



Dr. S. K. Reddy
Centre for Computational
and Data Science

