



Quality Improvement Programme (QIP)

Computationally Designing of Materials for Materials Genome

March 1-6, 2021

Organized by

Department of Chemistry

Indian Institute of Technology Indore



Course Overview

The Quality Improvement Program is organized to provide an introduction to computational modelling of materials. The comprehensive course will guide participants to design and investigate materials for novel applications. The objective of this course is to give insights into computational methods practiced for understanding various properties of materials and their experimental utilizations. The topics cover density functional theory, molecular dynamics and machine learning methods for developing material designing strategies. The course will illustrate how computational simulations can be used for better understanding of materials and guide the search for new promising methodologies. Optimizing material properties for energy related applications would be given special emphasis during the course. This QIP is in line with various GoI initiatives such as Make in India, Aatmanirbhar Bharat, Skill India, Start-up India, Digital India, AMRUT, so on and so forth.

Registration Process

For online registration, [click here](#)

Note :

- Registration in the course should be completed by **5pm, February 27, 2021.**
- Notification of acceptance of registration and the detailed schedule will be sent via email by **February 28, 2021.**

Eminent Speakers



Prof. Anoop Ayyappan
IIT Kharagpur



Prof. Md. Ehesan Ali
INST Mohali



Prof. Saurabh Ghosh
SRM University
Chennai



Prof. Sudeshna Chattopadhyay
IIT Indore



Prof. Sudip Chakraborty
IIT Indore



Prof. Biswarup Pathak
IIT Indore

Important Lectures

Theme 1: Computational methods and designing

Theme 2: Designing of Materials for Energy and Environmental Remediation

Theme 3: Programming for computational sciences

Theme 4: Design of multiferroic materials by combined effort of first principles calculations, machine learning and materials database

Theme 5: Molecular Dynamics Simulations: Algorithms and Applications in Protein Dynamics and Materials Designing

Theme 6: Materials Modelling for Energy Scavenging: A Computational Roadmap

Tutorials

Course Fees

No registration fee for faculty participants from AICTE approved colleges and institutes

Participants from non-AICTE institutes

- ❖ Rs. 7,000* (for industry personnel)
- ❖ Rs. 5,000* (for faculty / scientist)
- ❖ Rs. 2,000* (for student)

*inclusive of service tax

Mode of payment

Bank Transfer

Beneficiary Name: Registrar IIT Indore

Bank Name: Canara bank

Branch: IIT Indore, Khandwa Road, Simrol, Indore

Account number: 1476101027440

IFS Code: CNRB0006223

SWIFT Code/BIC: CNRBINBBISG

Course Registration

- ❖ Number of seats are limited
- ❖ Online link will be provided for the registered participants prior to the FDP
- ❖ Certificates will be issued for the registered participants
- ❖ All relevant queries should be directed through e-mail to: mkushwaha@iiti.ac.in

Course Coordinator

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