



SERB Sponsored Karyashala Event

## WINTER SCHOOL ON

# QUANTUM CHEMICAL CALCULATIONS AND MOLECULAR DYNAMICS SIMULATIONS

January  
4 - 10, 2024



## ABOUT KARYASHALA

Karyashala is a noble endeavor of Government of India under Accelerate Vigyan Scheme to improve research productivity of promising B.Tech, M.Tech. and Ph.D. students from universities and colleges through high-end workshops on specific themes. These events are sponsored by Science and Engineering Board (SERB). These workshops aim to equip the participants with specialized research skills.

## COURSE DETAILS

The course aims at focusing on the techniques of molecular simulation/modeling adopted by chemists, physicists and chemical engineers. These techniques have currently been used to predict the thermodynamic properties of pure component/real mixtures, which is a prerequisite for the design and simulation of chemical, biochemical, and environmental systems. It gives a route for the calculation of equilibrium and dynamic properties of the system such as: phase equilibria, transport coefficients and catalytic processes. Research scholars will highly benefit from the exposure due to the hands on session associated with these modules.

## TOPICS COVERED

Density Functional Theory; Molecular Dynamics Simulations; Monte Carlo Simulations; Periodic DFT and Ab-initio-Molecular Dynamics

## REGISTRATION

There is no registration fee. Travel, food and on-campus accommodation expenses will be reimbursed for the students as per DST-SERB Guidelines

## IMPORTANT INFORMATION

**The Last Date for Application :** 10th December 2023

**VENUE:** Department of Chemical Engineering, IIT Guwahati

## CONTACT



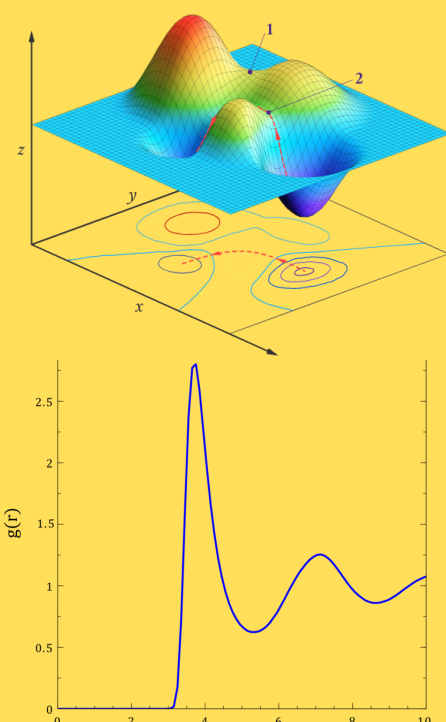
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## HOW TO APPLY

Interested candidates may visit the following [link](#) and fill up necessary information to register themselves. Additionally, the candidates need to submit the following three documents in PDF format to [tamalb@iitg.ac.in](mailto:tamalb@iitg.ac.in)

- **Endorsement cum No Objection Certificate** in the letterhead of the applicant's institute. This certificate is to be submitted in the prescribed format and is available [here](#).
- An **Undertaking Form** duly filled and signed by the candidate. The undertaking form can be downloaded from [here](#).
- A **Short CV** indicating the candidate's CPI/Marks till date

## WHO CAN ATTEND

- The Event is open to BTech(Final Year), MSC, MTech and PhD students
- The event will be physically conducted at IIT Guwahati. There are only 25 seats. The theory lectures are associated with practical sessions. Preference will be given to applicants at the early stage of their Ph.D study.
- Selection of Candidates shall be made by the Committee comprising of the Host Institute Resource Persons and shall be communicated in due course of time.

