

## Workshop on In-Silico Quantum Modeling Studies

23rd-27th February 2026



## ABOUT THE WORKSHOP

IUAC is organizing a workshop on In Silico Quantum Modeling Studies to equip researchers, particularly in materials science, with essential computational techniques for studying quantum systems. It features lectures by eminent experts on topics including band structure, density functional theory, modelling of polymers and high pressure, low-dimensional, energy and biological materials, the interface between theory and experiment, and new computing technologies. The lectures are complemented by hands-on computing lab sessions. The software for density functional theory calculations will be Quantum Espresso package. Familiarity with Linux Operating System is a requirement for the hands-on sessions. The participants are required to bring their own laptops with Linux installed on them.

## Tentative List of Topics to be covered

- Magnetism in 2D materials
- 2D based materials for hydrogen storage
- Thermoelectric materials
- Molecular dynamics of biomolecules
- Machine learning in materials science
- Defects in 2D materials
- DFT level simulations for battery projects applications

## Tentative List of Speakers\*

- Prof. Ravindra Pandey MTU, USA
- Dr. Puspamitra Panigrahi, HITS Chennai
- Dr. Ashok Kumar, Central University Punjab, Bhatinda
- Dr. Dr. Mohan Verma Shri Shankarayacharya Technical Campus, Bhilai
- Dr. Keshav Rao Shri Shankarayacharya Technical Campus, Bhilai
- Dr. B. K. Sahu, IUAC New Delhi
- Mr. Abhishek Kumar, IUAC New Delhi
- Dr. Mukesh Jakhar IUAC New Delhi

(\* will be updated soon)

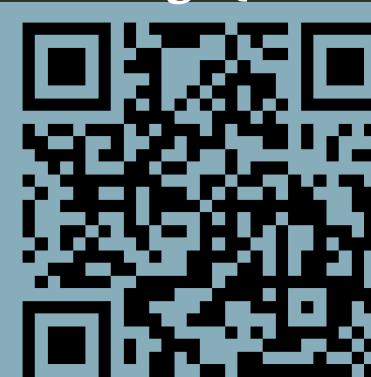
## REGISTRATION FEE

A registration fee of Rs. 2000 per participant, which covers the registration kit and local hospitality, is required to be deposited by the shortlisted candidates.

## IMPORTANT DATES

Registration Opens	24th December 2025
Registration Closes	12th January 2026
Intimation of selection	16th January 2026
Workshop	23rd-27th February 2026

Scan the following QR code to register:



Note: Travel support & shared accommodation will be arranged for outstation participants.

## VENUE:

Seminar Hall,  
Inter-University Accelerator Centre  
Aruna Asaf Ali Marg  
Vasant Kunj, Delhi-110067

## ORGANIZING COMMITTEE

PROF. RAVINDRA PANDEY, DR. BHUBAN KUMAR SAHU, DR. AMBUJ TRIPATHI, PROF. SIKHA VERMA, DR. SAIF AHMAD KHAN, MR. ABHISHEK KUMAR, DR. MUKESH JAKHAR