

Workshop on *in-silico* Quantum Modelling Studies

22rd February-27th February 2026
Inter-University Accelerator Centre, New Delhi

Program Schedule

22 th February 2026 (Sunday) (Pre-Workshop Training)		
11.00 onwards Registration		
12.30-13.30	Lunch	
13.30-15.00	Introduction to Linux	Dr. Mohan L. Verma, Shri Shankaracharya Technical Campus-SSGI, Bhilai / Dr. Ashok Kumar, Central University of Punjab, Bathinda/ Dr. Mukesh Jakhar, IUAC, Delhi
15.00-15:45	An Introduction to High Performance Computing (hybrid)	Mr. Abhishek Kumar IUAC New Delhi
Tea Break		
16:15-17:15	Job submission Methodology and demonstration (hybrid)	Mr. Abhishek Kumar and Dr. Mukesh Jakhar, IUAC, Delhi
19:30	GET TOGETHER for participants' introduction	
20:30	Dinner	

23 rd February 2026 (Monday)		
09.30-09:30 Registration		
09.30-10.00	Introduction to the Workshop	Prof. Ravi Pandey, Michigan Tech University, USA + IUAC team (Dr. Bhuban Sahu, Dr. Saif Ahmad Khan, Dr. Ambuj Tripathi)
10.00-11.00	An Insight into Materials Physics - Experiment, Theory and Application	<i>To be updated soon</i>
Tea Break		
11.30-12.30	Introduction to Density Functional Theory	Dr. Mukesh Jakhar, IUAC, Delhi
12.30-13.00	How good is DFT?	Prof. Ravi Pandey, Michigan Tech
13.00-13.30	Param Rudra - HPC facility at IUAC	Dr. Bhuban Kumar Sahu, IUAC, Delhi
Lunch		
14.30-15.00	Band Structure, Density of States (DOS) and Carrier	Dr. Sujata, Central University of Panjab, Bhatinda

	mobility Calculations	
15.00-16.30		Lab - Assignment 1
Tea Break		
17.00-18.00		Lab - Assignment 1
20:00		Dinner
24th February 2026 (Tuesday)		
09.30-10.30	Materials Physics - Experiment and Theory	Prof. Ambesh Dixit, Indian Institute of Technology Jodhpur
10.30-11.30	DFT -Photocatalytic Applications	Dr. Ashok Kumar, Central University of Punjab, Bathinda
Tea Break		
12.00-12.45	Energy Materials in Various Prospects	Dr. Mohan Verma, Shri Shankaracharya Technical Campus-SSGI, Bhilai
12.45-13.30	Thermoelectric Materials	Dr. Manish Kumar, JNU, Delhi
Lunch		
14.30-15.30		Lab - Assignment 2
Tea Break		
16:00 - 17:00		Lab - Assignment 2
17.00-18.00		Lab - Assignment 3
20:00		Dinner

25th February (Wednesday)		
09.30-10.30	Solid State Hydrogen Storage	Prof. Kavita Joshi, NCL, Pune
10.30-11.30	DFT - Sensing	Dr. Puspamitra Panigrahi, Hindustan Institute of Technology and Science, Chennai
Tea Break		
12.00-12.45	Device - Interconnects	Dr. Santhibhushan, IIIT Prayagraj
12.45-13.30	Cathode Material Simulations for Li and Na ion Batteries	Dr. Amreen bano, TCGCREST, Kolkata
Lunch		
14.30-15.30		Lab - Assignment 3

Tea Break	
16.00-18.00	Lab - Assignment 4
Trip to Qutub Minar	

26 th February (Thursday)		
09.30-10.30	Molecular dynamics simulations and GPU applications	Dr. Anupam Nath Jha, Tezpur University, Tezpur
10.30-11.30	Computational Biology	Dr. Vinod Jani, CDAC, Pune
Tea Break		
12.00-12.45	DFT- Polymer	Prof. Ravi Pandey, Michigan Tech
12.45-13.30	Machine Learning in Materials Science	Dr. Ashok Kumar, Central University of Punjab, Bathinda
Lunch		
14.30-15.30	Lab assignment - 4	
Tea Break		
16:00-18.00	Lab assignment - 4	
20:00	Director's Dinner	

27 th February 2026 (Friday)		
09.30-10.30	Radiation Physics	Dr. Arghya Chattaraj, BARC
10.30-11.30	Radiation Defects	Dr. Mukesh Jakhar, IUAC
Tea Break		
12.00-13.00	2-slides presentation - Participants	
13.00-13.30	"Open Forum"	
Lunch		

Resource Persons for Lab-sessions: Mukesh Jakhar, Mohan Verma, Ashok Kumar, Ravi Pandey, Nayab Kumar, Sajal Biswas, Sujata, Abhishek Kumar

Please note:

1. The registration desk will be in the lounge area of the main building
2. Lab sessions/hands-on sessions will be in the seminar hall/Ph D Teaching Room (304 of the main building)
3. A get-together and a Two-slides presentation will be in the seminar hall