Winter School on Chemistry with Computers: Theory and Computations

प्रतिष्ठित संस्थान
INSTITUTION OF EMINENCE

OBJECTIVES

Lectures on classical and quantum computational chemistry at atomic and micro-level; *ab initio* quantum chemistry & physics, potential energy surfaces, dynamics and algorithms; machine learning algorithms (AI/ML); Monte Carlo and molecular dynamics simulations; Molecular mechanics and docking with applications on Reaction Mechanisms, Drug discovery, Material design, Excited Molecular State & Spectroscopy, Solvation dynamics, Adsorption isotherms, Protein structure and dynamics.

Hands-on training on ***Gaussian, Schrödinger, Gromacs, RASPA and Orange***

Registration fees

Rs. 15,000/+ 18% GST
(with accommodation and food for external participants)
Rs. 5,000/+ 18% GST (with food for University of Hyderabad students)



Date: 7th – 19th December, 2026
Time: 10:00 AM – 5:00 PM
Venue: School of Chemistry, University of Hyderabad

Registration deadline: 25.11.2026

Registration https://forms.gle/mjRoW8itf1uX58KLA

Website http://chemistry.uohyd.ac.in/

Target Participants:
PhD scholars, Postdocs, Faculty, MSc students

ORGANISED BY
NRCC, SCHOOL OF CHEMISTRY, UNIVERSITY OF HYDERABAD

Contacts for accommodation: ugcnrcsc@gmail.com,
any other information about the workshop: susanta.mahapatra@uohyd.ac.in, akssc@uohyd.ac.in, jovanjose@uohyd.ac.in

CONVENOR
Prof. S. Mahapatra, UoH,
Faculty, School of Chemistry
(Local organizing committee)

Winter School on Chemistry with Computers: Theory and Computations

प्रतिष्ठित संस्थान
INSTITUTION OF EMINENCE

Resource Persons

Prof. Krishnan Raghavachari
Indiana University, USA

Prof. S.R. Gadre
University of Pune

Prof. Sourav Pal
Ashoka University

Prof. Swapan K. Ghosh
BARC, Mumbai

Prof. Pratim Chattaraj
IIT Kharagpur

Prof. Satrajit Adhikari
IACS, Kolkata

Prof. Harjinder Singh
IIIT Hyderabad

Prof. Deva Priyakumar
IIIT Hyderabad

Prof. G. S. Vaitheeswaran
University of Hyderabad

Prof. Sanjay Kumar
IIT Madras

Prof. V. Subramanian
IIT Madras

Prof. Jagannath Mondal
TIFR Hyderabad

Prof. Soumya Ghosh
TIFR Hyderabad

Prof. Sabyashachi Mishra
IIT KGP

Prof. Ayan Dutta
IACS, Kolkata

Prof. Suryoday Prodhan
BITS Hyderabad

Prof. Naiwrit Karmodak
Shiv Nadar University

Prof. Rudraditya Sarkar
GITAM, Hyderabad

Prof. Rajgopal Rao
IIT Patna

Prof. Rajgopala Reddy
CUR

Dr. Tanmoy Mondal
KL University, Hyderabad

Prof. Kalidas Sen
University of Hyderabad

Prof. Lalitha Guruprasad
University of Hyderabad

Prof. S. Mahapatra
University of Hyderabad

Prof. Debashis Barik
University of Hyderabad

Dr. Manju Sharma
University of Hyderabad

Dr. K. V. Jovan Jose
University of Hyderabad

Topics



