

Winter School on Chemistry with Computers: Theory and Computations

Objectives

- ❖ Lectures and Hands-on training on quantum chemistry, quantum computing and quantum algorithms, AI/ML for molecules and materials, molecular dynamics, and molecular docking and drug discovery

 **Date:** 7th – 19th December, 2026

 **Time:** 10:00 AM – 5:00 PM

 **Venue:** School of Chemistry,
University of Hyderabad

Registration deadline: 15.11.2026

 **Target Participants:**
PhD scholar, Postdocs,
Faculty, MSc students

Registration

<https://forms.gle/WWsPLjKLfAT6xh4t9>

Website

<http://chemistry.uohyd.ac.in/>



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

Registration fees

Rs. 25,000/+ 18% GST

(with accommodation and food for external participants)

Rs. 8,000/+ 18% GST (with food for University of Hyderabad students)



ORGANISED BY

**NRCC, SCHOOL OF CHEMISTRY,
UNIVERSITY OF HYDERABAD**

CONVENOR

Prof. S. Mahapatra, UOH,

Faculty, School of Chemistry
(Local organizing committee)



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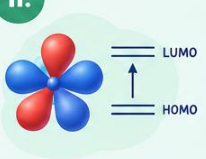


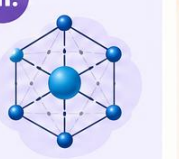
Resource Persons

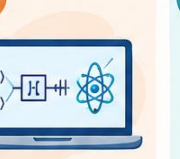
Prof. Debashis Mukherjee, IACS, Kolkata	Prof. Krishnan Raghavachari Indiana University, USA	Prof. Sourav Pal Ashoka University	Prof. Satrajit Adhikari IACS, Kolkata	Prof. Kalidas Sen University of Hyderabad	Prof. S.R. Gadre University of Pune	Prof. T.P. Radhakrishnan University of Hyderabad
Prof. G. Narahari Sastry IIT Hyderabad	Prof. Harjinder Singh IIIT Hyderabad	Dr. Madhavi Sastry Hyderabad	Prof. Deva Priyakumar IIIT Hyderabad	Prof. G. S. Vaitheeswaran University of Hyderabad	Prof. V. Subramanian IIT Madras	Prof. Lalitha Guruprasad University of Hyderabad
Prof. S. Mahapatra University of Hyderabad	Prof. Debashis Barik University of Hyderabad	Prof. Suryoday Proadhan BITS Hyderabad	Prof. Rajgopal Reddy CUR	Prof. Soumya Ghosh TIFR Hyderabad	Prof. Jagannath Mondal TIFR Hyderabad	Prof. Sanjay Kumar IIT Madras
Prof. Ayan Dutta IACS, Kolkata	Prof. Debashree Ghosh IACS, Kolkata	Prof. Naiwrit Karmodak Shiv Nadar University	Prof. Rudraditya Sarkar GITAM, Hyderabad	Prof. Rajgopal Rao IIT Patna	Prof. Shrabani Taraphder IIT KGP	Dr. Tanmoy Mondal KL University, Hyderabad
				Prof. Jovan Jose University of Hyderabad	Prof. Sabyashachi Mishra IIT KGP	

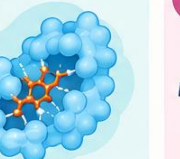
Topics

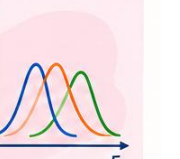
i. 
Fundamentals of Quantum Chemistry

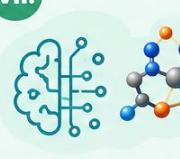
ii. 
Electronic Structure Calculations, including Ab Initio Methods

iii. 
Symmetry and Group Theory

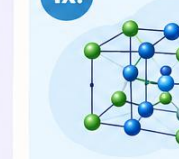
iv. 
Quantum Computing and Quantum Algorithms

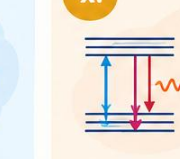
v. 
Computational Approaches to Molecular Docking and Drug Discovery

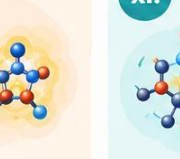
vi. 
Statistical Mechanics: Fundamentals and Applications

vii. 
AI/ML for Molecules and Materials

viii. 
QM/ML and Monte Carlo Simulations

ix. 
Computational Studies of Molecules in Crystals

x. 
Computational Chemistry of Excited States and Photochemical Processes

xi. 
Molecular Dynamics and Free-Energy Calculations

