One-Day Symposium

on

FRONTIERS IN COMPUTING IN CHEMISTRY:

FROM MOLECULAR MECHANISMS TO COMPLEX SYSTEMS

28th September 2026

CSB Seminar Hall & Harish-Chandra Seminar Hall,
IISER Thiruvananthapuram

Organized by

Center for High-Performance Computing, IISER Thiruvananthapuram

Speakers

Arun Venkatnathan, *IISER Pune*

Investigating Battery Electrolytes: What Insights Can Quantum Chemistry and (ab initio) Molecular Dynamics Simulations Offer?

Debashree Chakraborty, *NITK Surathkal*

Effect of Neutral Crowders on Alpha-Synuclein Aggregation Kinetics

Ganapathy Vaitheeswaran, *University of Hyderabad*

From Molecular Insulator to Metal: Pressure-Driven Electronic Reconstruction in Iodanil

Jagannath Mondal, *TIFR Hyderabad*

Integrating Artificial Intelligence with Biomolecular Simulations

Rajib Biswas, *IIT Tirupati*

The Aqueous Urea Paradox: Intact Water Structure yet Retarded Dynamics

Suman Chakrabarty, *SNBNCBS, Kolkata*

Navigating Pathways in Free Energy Landscape: Adaptive (Machine) Learning Strategies Towards Rare Event Kinetics

Swati Bhattacharya, *IIT Bombay*

A Second-Long Trajectory of the TRP-Cage Peptide Generated Using a KMC Model Derived from Molecular Dynamics