

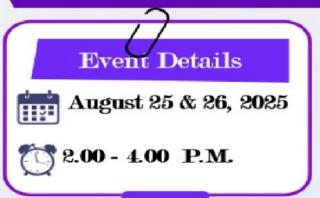


# DEPARTMENT OF CHEMISTRY

organizes

## Two-Day Virtual Workshop on Computational **Chemistry**

Modern Tools and Applications in Molecular Modeling and Simulation



#### **Resource Person**





Registration link https://forms.gle/QejAjXM7t7yVaPGc7

#### Dr. NIVEDITA ACHARJEE

Associate Professor Department of Chemistry, Durgapur

Government College, West Bengal

### Objectives of the event

- Equipping with practical skills in applying computational chemistry tools to study > selectivity, mechanisms, kinetics, and biological significance of chemical reactions.
- Utilizing the PASS Online Portal for predicting bioactivity of organic compounds and analyzing the results.
- Applying Avogadro software for regular teaching, learning, and research projects.
- Developing skills in conducting literature surveys of research articles and reviews to identify bioactive compounds.
- Training in Gaussian and Gauss View software for: optimizing molecular structures, calculating Frontier Molecular Orbital (FMO) energies, exploring spectroscopic properties, and designing computational projects.
- Applying Multiwfn software to analyze electron density, molecular orbitals, and chemical reactivity descriptors.
- Using visualization tools such as UCSF-Chimera and Visual Molecular Dynamics (VMD) to study molecular structures and dynamics.

Presided By Rev. Sr. Dr. Victoria Principal