Hands-on Computational Chemistry workshop

Molecular Modelling and DFT Applications

Organized by Department of Chemistry

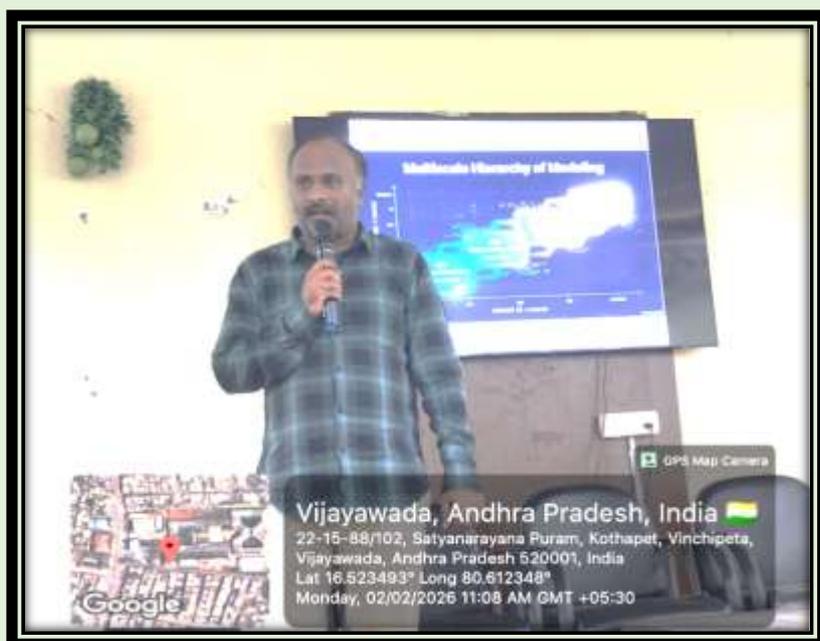## Date: 02nd February to 06th February 2026

The PG Department of Chemistry organized a **five-day (2-2-2026 to 6-2-2026) workshop on Molecular Modelling and DFT Applications** for M.Sc. Organic and Analytical Chemistry students. **Prof. Mahesh Ravva from SRM University** served as the Resource Person for the workshop."

Day 1: Introduction to Computational Chemistry

The workshop began with an inaugural session followed by an introduction to computational chemistry and molecular modelling. Prof. Mahesh Ravva explained the importance of computational tools in modern chemical research, drug design, and material science. Students were introduced to molecular visualization software and basic modelling concepts.

Day 2: Fundamentals of Molecular Modelling

On the second day, the resource person discussed force fields, energy minimization, and molecular geometry optimization. Students performed hands-on exercises using molecular modelling software to construct and optimize simple organic molecules. The session helped students understand molecular stability and structural parameters.

Day 3: Introduction to Density Functional Theory (DFT)

The third day focused on the basic principles of Density Functional Theory (DFT). The resource person explained quantum mechanical approaches, basis sets, and functionals. Students learned how DFT calculations are used to predict molecular properties such as energy, dipole moment, electronic structure, UV absorption and IR vibrations.

Day 4: Practical Applications of DFT

On the fourth day, students performed DFT calculations using computational chemistry software. They learned to interpret output data, including HOMO–LUMO analysis, molecular orbitals, and energy calculations. The session emphasised the application of DFT in organic and analytical chemistry research.

Day 5: Advanced Modelling and Valedictory Session

The final day covered advanced topics like NMR spectra and solvent effects on the molecules, and other applications of molecular modelling in research.

Students interacted with the resource person to clarify doubts and discuss research applications. The workshop concluded with a valedictory session, where participants shared feedback about their learning experience.

Finally programme ends with certificate distribution to the student participants.

Vijayawada, Andhra Pradesh, India
22-15-88/102, Satyanarayana Puram, Kothapet, Vinchipeta,
Vijayawada, Andhra Pradesh 520001, India
Lat 16.523522° Long 80.612353°
Friday, 06/02/2026 03:05 PM GMT +05:30

Vijayawada, Andhra Pradesh, India
22-15-88/102, Satyanarayana Puram, Kothapet,
Vinchipeta, Vijayawada, Andhra Pradesh 520001, India
Lat 16.523476° Long 80.612331°
Friday, 06/02/2026 03:21 PM GMT +05:30

FALICITATION TO THE CHIEF GUEST