



Module PMRF-ISSS031/IV/2025

Quantum Chemistry

Name of the PMRF student

Ritwika Chatterjee

Details of the content of the module

Required background of the students taught

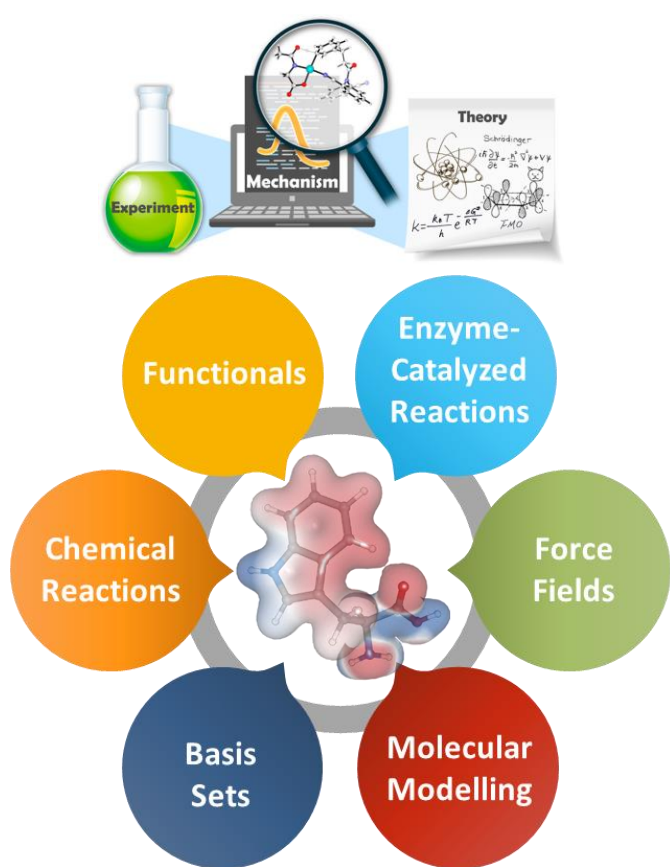
UG in chemistry

• Basic concepts of Quantum Chemistry

1. Operators
2. Particle in a box
3. Rigid rotor
4. Variational Principle
5. Perturbation Theory
6. Hartree-Fock theory
7. DFT
8. Hartree-Fock Theory

• Concepts of Computational Modelling

Potential Energy Surface, Born-Oppenheimer Approximation, Stationary Points, Geometry Optimization, Normal-Mode Vibrations



Schedule of the module

Start Date: **06/05/2025**

End Date: 07/06/2025 (tentatively)

Class Timing: Tuesday and Saturday, 6 PM

Meeting link : Will be shared later

[Link](#)

Contact email ID: issforum@gmail.com

Registration link:

<https://forms.gle/rFUiEPCpFBYqBeY19>