



Module PMRF-ISSS027/III/2025

Computational Chemistry

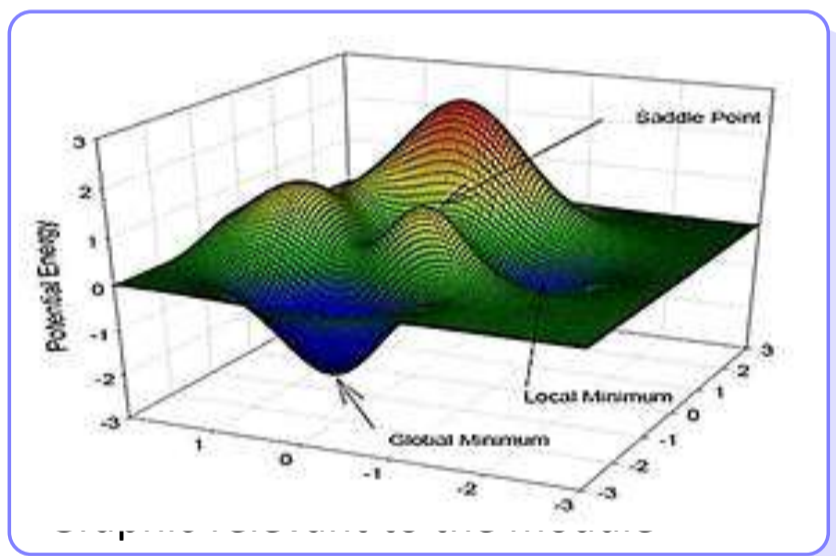
Name of the PMRF student

SAPNA

Required background of the students taught

B.Sc in Chemistry

M.Sc in Chemistry (not mandatory)



Details of the content of the module

Live lecture sessions on Computational Chemistry:

What is computational Chemistry ?

The concept of Potential Energy Surface

- Stationary point
- Born Oppenheimer principle
- Geometry Optimization
- Stationary points and normal mode of vibrations

Introduction of Quantum Mechanics in computational Chemistry

- Huckel theory
- Extended huckel theory

Introduction of Basis set and functionals

- Slater type basis set
- Gaussian type basis set
- Functionals

Schedule of the module

Start date: 20th March 2025

End date(tentative): 20rd May 2025

Live lectures on Monday & Saturday: 9:00 AM – 10:00 AM

Meeting link : Will be shared later

[Link](#)

Contact email ID: issf.forum@gmail.com

sapna2022@iisc.ac.in

Registration link:

<https://forms.gle/wm4nuV2VcGP32bbW9>