PMRF-ISSS Teaching Programme

Prime Minister Research Fellowship students' teaching requirement facilitated by the Institute of Smart Structures and Systems

Module PMRF-ISSS091/IV/2025

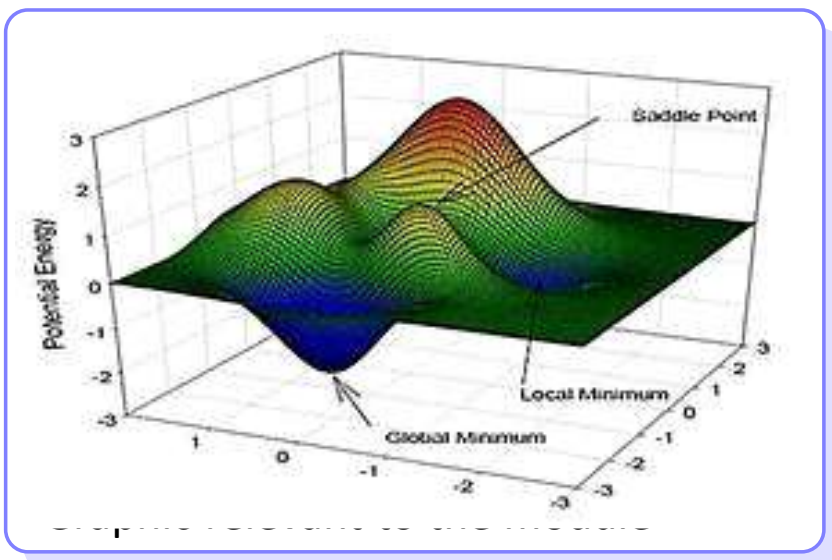
Computational Chemistry

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 points
- Born Oppenheimer principle
- Stationary points and normal mode of vibrations

Introduction of Quantum Mechanics in computational Chemistry

Ab initio calculations

- Basic principle of Ab initio method
- Basis set
- Post Hartree Fock Calculation – electron correlation

Semiempirical Calculations

- CNDO, INDO and NDDO method

Density Functional Calculations

- Basic principles
- Application

Schedule of the module

Start date: 10th sept 2025

End date(tentative): 10rd dec 2025

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

Meeting link : Will be shared later

Link

Contact email ID: isss.forum@gmail.com

sapna2022@iisc.ac.in

Registration link:

https://forms.gle/zSzQQNpEFPjLfVaH7