PMRF-ISSS Teaching Programme

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

Module PMRF-ISSS046/II/2024

Basics of Computational Chemistry

Name of the PMRF student

Ritwika Chatterjee

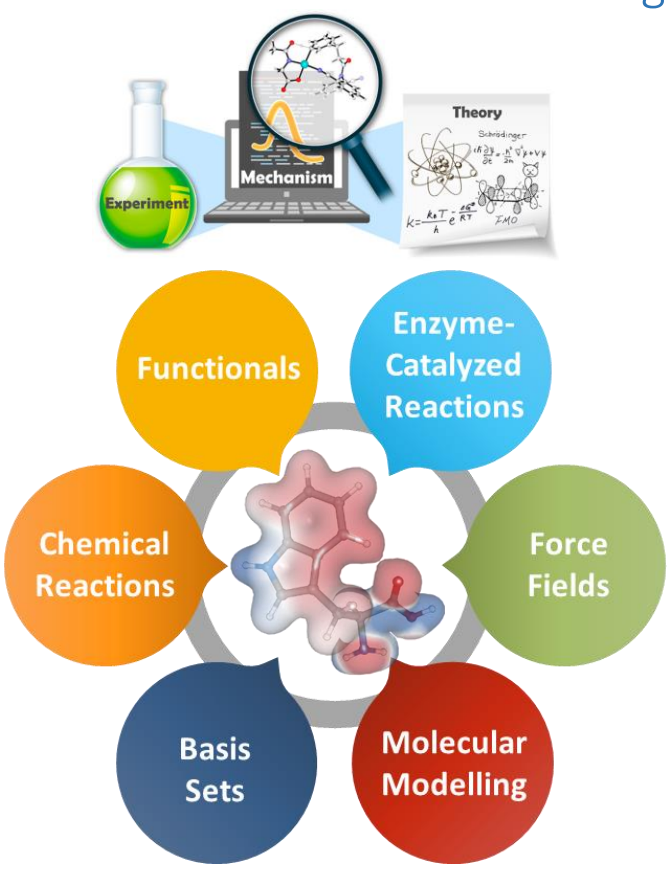
Required background of the students taught

Basics of Quantum Mechanics is desired

3rd/4th year UG or PG students

Online session coordinator

Will be chosen from the list of registrants



Details of the content of the module

- **Concepts of Computational Modelling**

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

- **Molecular Mechanics**

  Basic Principles, Force Fields, Basics of Molecular Dynamics Simulations

- **Ab Initio Methods**

  Hartree-Fock Method, Basis Sets

- **Density Functional Theory**

  Foundation, Kohn-Sham Self-consistent Field Method, Exchange-correlation Functionals

- **Hybrid Quantum/Classical Methods**

  Applications in Enzymatic Systems

Schedule of the module

Start Date: **08/03/2024**

End Date: 30/04/2024 (tentatively)

Class Timing: Tuesday and Friday, 10 AM (1hour)

Meeting link : Will be shared later

Contact email ID: isss.forum@gmail.com

Registration link: Click HEREor, scan the QR code