PMRF-ISSS Teaching Programme

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

Module **PMRF-ISSS058/2024**

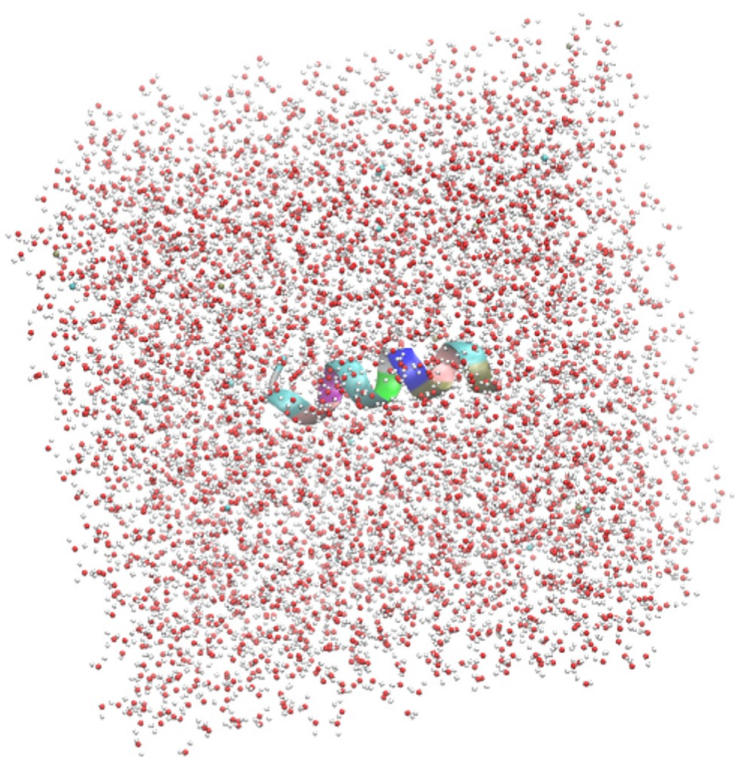
Introduction to Molecular Dynamics

Name of the PMRF student

Amar Krishna Gopinath

Required background of the students taught

Students in the undergraduate or post graduate courses, preferably, Chemical engineering / Physics / Chemistry, and with a background in thermodynamics



Details of the content of the module

This module is targeted to be a beginner's guide to molecular dynamics. The student shall be guided on the key techniques required to build a molecular dynamics simulation from scratch.

The module is divided into four sections:

- **Introduction to statistical mechanics**
  - Ensemble theory- discussion of various types of ensembles and relation to thermodynamics properties
  - Lagrangian and Hamiltonion approaches for obtaining equations of motion
- **Basics of molecular dynamics simulations**
  - Modeling molecular interactions- description of forcefields in molecular dynamics
  - Force calculation algorithm
  - Computation of thermodynamic and transport properties
- **Advanced techniques**
  - Molecular dynamics extended to other ensembles: use of thermostats and barostats
  - Particle Mesh Ewald technique for multibody electrostatics
- **Free energy techniques**
  - Free energy perturbation
  - Umbrella sampling

Schedule of the module

Session start date: 13 April 2024

Session end date: 29 June 2024

Schedule: Recorded lectures shall be uploaded every Saturday and Sunday

Meeting link : Will be shared later

Link:

Contact mail ID: amargopinath@iisc.ac.in

Registration link: https://forms.gle/ftYQDDz[redacted]