



PH322 Jan 3:0

Molecular Simulation

Instructor

Prabal Kumar Maiti

Email: maiti@iisc.ac.in

Teaching Assistant

Mounika Gosika

Email: mounika.gosika@gmail.com

Department: Physics

Course Time: Wed., Fri., 11:00-12:30PM

Lecture venue: Multi-Media Room, New Physical Sciences Building

Detailed Course Page: <http://www.physics.iisc.ernet.in/~ph322>

Announcements

Brief description of the course

Students aiming to pursue research in simulation of soft matter and hard matter

Prerequisites

First course in Quantum Mechanics and Statistical Mechanics

Syllabus

Introduction Molecular dynamics, Various schemes for integration,

Inter and Intra molecular forces, Introduction to various force field,

Methods for partial atomic charges, Various ensemble (NVE, NVT, NPT, NPH),

Hard sphere simulations, water simulations, computing long range

interactions

Various scheme for minimization: conjugate gradient, steepest descent.

Monte Carlo Simulations, Rigid Body Monte Carlo, Various sampling methods,

Particle based MC simulations, Biased Monte Carlo. Free energy calculations,

Umbrella sampling, Free energy perturbation,

Applications: Nanotube simulations, Liquid crystal simulations,

Introduction to biomolecule simulations

Course outcomes

Writing basic MD and MC code. Understand advanced sampling, Able to get started with the research in this area

Grading policy

20% for assignments

20% for mid term

30% for project

30% for final

Assignments

Resources