PHYS-235: Molecular Simulation

This course will introduce students to the range of methods currently being used to simulate the behavior of matter at the molecular scale. Basic methods for equilibrium Monte Carlo and molecular dynamics simulations will be described, including techniques for generating different ensembles and calculating free energies and phase equilibria. Assignments will involve applying these methods to sample problems. Papers of related work will be discussed.

Credits: 3

Program: Physics

1 2023-2024