CHEM 3353 : Computational Chemistry

Introduction to the main areas of computational chemistry including theoretical background, algorithms and implementation, and applications in molecular modeling. Major topics include potential energy surfaces, molecular mechanics, continuum methods, docking, molecular dynamics, quantum mechanics, basis-sets, and post Hartree-Fock methods. This hands-on course will also provide experience in scientific programming in Python, and use a variety of free software tools for molecular visualization and simulation. No prior programming experience is assumed.

Credits 3

Course ID

009597

Requisites

CHEM 3353 Prerequisites (with a grade of 'C' or better): CHEM 1342/1142, MATH 1432

Semester Offered

Spring semester, even years