CHEM 267 – Special Topics in Physical Chemistry
Introduction to Molecular Modeling

Summary

Do you know how to create and view a molecular structure in the computer? Have you thought about the technology behind a chemical database? Do you want to know how it feels to see a molecule in Virtual Reality? Do you know how to design molecules that may work as new medicines or materials? Are you **(Chemical)** **We have so much to introduce, not just theory but computational experiments …**

We will explore the techniques and applications of molecular modeling and computational chemistry. This course highlights how to model different molecules (from small molecules to macromolecules, polymers, assemblies, frameworks, etc.) in computers and how to calculate their properties and reactions with modern computational technology. Computational and informatics approaches are introduced from a practical aspect, in conjugation with special topics such as computer-aided drug design and big chemical data. This course is targeted at advanced graduate/undergraduate levels, with the goals to (i) strengthen the understanding of the molecular sciences and (ii) introduce useful modeling skills for solving research problems.

Some of the introduced computational programs are free for academic users — feel free to bring your laptop to classes. A powerful workstation in the Li group will be provided for some group exercises.

Prerequisites
‹   N/A

Textbooks
Given the fast development of computational chemistry, it is impossible

Topics

Learning Objectives