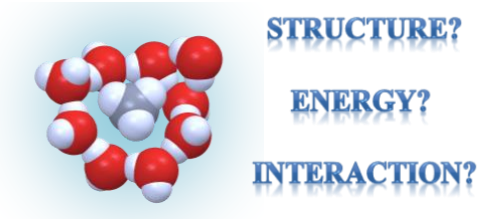
CHEM 267 – Special Topics in Physical Chemistry

Introduction to Molecular Modeling



Time: 1:15-2:30 PM TR

Room: VOTEY 254

Lecturer: Jianing Li (jianing.li@uvm.edu, Innovation E348)

Office Hour: TBA

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 prepared for the era of "Big (Chemical) Data"? — **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.

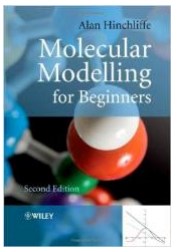
Some of the introduced computational programs are free for academic users — feel free to bring your laptop to classes. A powerful workstation in the Li group will be provided for some group exercises.

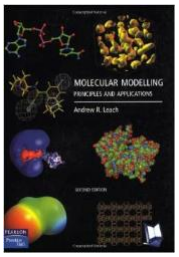
Prerequisites

- N/A

Textbooks

Given the fast development of computational chemistry, it is impossible to find a textbook with all the up-to-date materials. While we are trying to implement mostly new materials, some materials are from books below:





- Molecular Modelling: Principle and Applications, 2nd Edition, by Andrew R. Leach.
- Molecular Modelling for Beginners, 2nd Edition, by Alan Hinchliffe.
- Big Data for Dummies, by Judith Hurwitz.
- Clusters for Dummies, by Ed Tittel.

Topics

Learning Objectives	Course Topics	Skills
Understanding chemical structures; applying the knowledge to build computer models & search for molecules	1D, 2D, & 3D depictions of molecular structures; chemical data & databases; basic machine learning	Use computer programs to build molecular models Create professional figures Search chemical databases
Understanding molecular motions & interactions; analyzing structure-based properties	Classical & modern views of chemical interactions & molecular motions	Analyze molecular interactions Run molecular simulations & quantum calculations
Applying knowledge & skills of molecular modeling; evaluating molecular properties determined by structures & energetics	Multiscale introduction of computational technologies & case studies	Apply molecular modeling to chemical problems Communicate modeling results

Week 1-3. **Computational Chemistry 101: Chemical Formats, Software Tools, and Supercomputing.**
Week 4-6. **Basic Small-Molecule Modeling.**
Week 7-9. **Basic Macromolecule/Supermolecule/Polymer Modeling.**
Week 10-13. **Applications.**
Note: Lecture numbers are very approximate.

Grading

- Tasks (70%)
- Attendance (5%)
- Project (25%)