CH 354M / 393L – Introduction to Computational Methods in Chemistry

(Unique: 50294 / 50484)

Time and Place: Spring 2024, Tu/Th 12:30-2:00, WEL 3.320

Instructor: Graeme Henkelman,
henkelman@utexas.edu
Office hours: after class and when you want them

Assistants: Sung Jung,
sunghjung3@utexas.edu

Outline:

1. Mathematical introduction: calculus, algebra, and concepts of computing.
2. Kinetics of coupled chemical reactions.
3. Numerical calculations reaction dynamics using classical mechanics.
4. Molecular vibrations and normal modes.
5. Use of random numbers in simulations and Monte Carlo methods.
6. Numerical calculations of quantum mechanical wavefunctions and energy levels.
7. Waves and wavepackets.
8. Quantum chemistry calculations of small molecules
9. Density functional theory calculations of materials
10. Independent project.

Course website: Lecture notes, homework assignments and supplementary material will be posted on the canvas course website.

Homework: A new homework assignment will be assigned approximately every two weeks. As the goal of this course is to learn how to apply computational chemistry to real life problems and as there are only a handful of realistic problems that can be solved with pencil and paper you will need to solve most of the homework problems numerically. While it is entirely up to you what software and/or programming language you use for this, I suggest that you consider using Mathematica, which is available free for CNS students through the website, https://www.ph.utexas.edu/software/. You can turn in your assignments through the canvas website. The notebook should have sufficient comments so that someone else can understand what you did. I can provide help with using Mathematica. I will further provide Mathematica sample files that will appear on the course website and contain examples of using Mathematica functions relevant for homework assignments.

Project: An independent project will be assigned mid-semester and due in the last weeks of class. The project will involve finding an article or another source (such as a textbook) describing a calculation related to chemistry. This could be the extension of a concept that we have discussed in class, or some other topic in computational chemistry that you are interested in. The project must involve a calculation of your own, either reproducing or extending the work done in your reference. Project topics should be discussed with the instructor before you begin. Each student will present their project to the class at the end of the semester, and turn in a written report at that time.

Grading: Homework: 60%; Project: 40%

Suggested Texts:

Frenkel and Smit, *Understanding molecular simulation: From algorithms to applications*
Allen and Tildesley, *Computer simulations of liquids*
Press et al., *Numerical Recipes*
Wolfram, *The Mathematica Book*