Chemistry 430: Simulation in Chemistry & Biochemistry Spring 2021

Class Meetings: Monday and Wednesday, Lecture, 11:00-11:50, Remote via Zoom
Friday, Laboratory Sessions, One Hour Sessions, 454 Louderman or Remote

Instructor: Jay Ponder (453 Louderman, 935-4275, ponder@dasher.wustl.edu)

Web Site: http://dasher.wustl.edu/chem430/

Objectives: Chemistry 430 explores a wide range of computational applications in molecular modeling, biochemistry and biophysics, including \textit{ab initio} and semi-empirical electronic structure theory, molecular mechanics, molecular dynamics simulation, coarse-grained models, electrostatic methods, biomolecular structure prediction and machine learning in molecular modeling.

A major component of the course consists of weekly laboratory sessions using software programs including VMD, Avogadro, Spartan, Q-Chem, Psi4, Gaussian, VMD, Chimera, Tinker, FFE, APBS, Modeller, AutoDock, SDA7 and others. Many of the lab exercises target proteins, nucleic acids and other biological structures.

Books: The book that most closely follows the course outline is Molecular Modeling by Andrew Leach. While not required, Leach’s book is a well-written introduction. Other useful books are listed below, and readings from these will be provided.

\textit{General Molecular Modeling:}

Molecular Modeling – Principles and Applications, 2\textsuperscript{nd} Ed., Andrew Leach, 2001
Molecular Modeling and Simulation, 2\textsuperscript{nd} Ed., Tamar Schlick, 2010
Introduction to Computational Chemistry, 3\textsuperscript{rd} Ed., Frank Jensen, 2017
Essentials of Computational Chemistry, 2\textsuperscript{nd} Ed., Christopher Cramer, 2004
Computational Chemistry, 2\textsuperscript{nd} Ed., Errol Lewers, 2010

\textit{Algorithms & Theory for Quantum Chemistry:}

Modern Quantum Chemistry, Attila Szabo & Neil Ostland, 1982 (reprinted by Dover)
Quantum Chemistry, 3\textsuperscript{rd} Ed., John Lowe and Kirk Petersen, 2006
Molecular Orbitals & Organic Chemical Reactions, Ian Fleming, 2010
The Theory of Intermolecular Forces, 2\textsuperscript{nd} Ed., Anthony Stone, 2013

\textit{Simulation & Biochemical Applications:}

Computer Simulation of Liquids, 2\textsuperscript{nd} Ed., M. P. Allen & D. J. Tildesley, 2017
Understanding Molecular Simulation, 2\textsuperscript{nd} Ed., Daan Frenkel & Berend Smit, 2002
Computational Biochemistry & Biophysics, Becker, \textit{et al}., 2001
A Guide to Biomolecular Simulations, Becker & Karplus, 2006

Other Info: Chemistry 430 is intended for advanced undergraduates and early graduate students wanting to learn modern computational and modeling approaches to chemical, biochemical and biophysical problems. A course in physical chemistry is recommended as background, but not required. Familiarity with computers to the level of writing scripts or small programs is recommended, but not required.
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Module 3: Electrostatics, Coarse Graining & Biomolecular Structure Prediction

Apr 12  Break Day – No Class
Apr 14  Protein Structure Prediction, Engineering & Design
Apr 16  Lab 10: Homology Modeling of a Lactate Dehydrogenase
Apr 19  Small Molecule & Protein Docking I
Apr 21  Small Molecule & Protein Docking II
Apr 23  Lab 11: Docking Indinavir to HIV Protease Using Autodock
Apr 26  Computing Binding Rate Constants via Brownian Dynamics
Apr 28  Introduction to Convolutional Neural Networks
Apr 30  Lab 12: Diffusional Association of the Barnase-Barstar Complex
May 4  Machine Learning in Computational Chemistry

May 13  Lab Reports & Take-Home Final Assignment Due