Chemistry 478: Molecular Modeling Spring 2014

Class Meetings: Monday and Wednesday, Lecture, 11:00am-Noon, 460 Laboratory Sciences
Friday, Laboratory Session, 11:00am-Noon, 460 Laboratory Sciences

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Web Site: http://dasher.wustl.edu/chem478/

Objectives: Chemistry 478 explores a wide range of techniques and applications in molecular modeling and computational chemistry, including *ab initio* quantum mechanics, semi-empirical MO theory, molecular mechanics, molecular dynamics simulation, coarse-grained models, electrostatic methods and biomolecular structure prediction.

Books: The book that most closely follows the course outline is Molecular Modeling by Andrew Leach. There are copies available in the WashU Bookstore and from online booksellers. While not "required", Leach is a well-written, useful introduction. Other good books are listed below, and readings from these will be provided.

Molecular Modeling: (emphasis on quantum chemistry)

Introduction to Computational Chemistry, 2nd Ed., Frank Jensen, 2007
Essentials of Computational Chemistry, 2nd Ed., Christopher Cramer, 2004
Molecular Modeling Basics, Jan Jensen, 2010

Molecular Modeling (emphasis on simulation and modeling)

Molecular Modeling – Principles and Applications, 2nd Ed., Andrew Leach, 2001
Molecular Modeling and Simulation, 2nd Ed., Tamar Schlick, 2010

Algorithms & Theory for Quantum Chemistry:

Modern Quantum Chemistry, Attila Szabo & Neil Ostland, 1982 (reprinted by Dover)
Quantum Chemistry, 3rd Ed., John Lowe and Kirk Petersen, 2006

Qualitative Molecular Orbital Theory:

Frontier Orbitals – A Practical Manual, Nguyen Trong Anh, 2007
Molecular Orbitals & Organic Chemical Reactions, Ian Fleming, 2010

Algorithms & Theory for Simulation:

Computer Simulation of Liquids, M. P. Allen & D. J. Tildesley, 1987
Understanding Molecular Simulation, 2nd Ed., Daan Frenkel & Berend Smit, 2002
The Theory of Intermolecular Forces, 2nd Ed., Anthony Stone, 2013

Other Info: Chemistry 478 is targeted at an advanced undergraduate level, but is also suitable for graduate students wanting background in modern computational and modeling approaches to chemical problems. A prior course in physical chemistry, or consent of the instructor is required. Some basic familiarity with computers (text editing, writing small scripts or programs) is highly recommended, but not required.

Module 1:	***ab Initio* and Semi-Empirical Quantum Mechanics**
Jan 13	Introduction to Molecular Modeling; Examples of Application Areas
Jan 15	Potential Energy Surfaces and Optimization Methods
Jan 17	Lab 1: Using Spartan, Gaussian, TINKER and the Cygwin shell
Jan 20	NO CLASS (Martin Luther King Day)
Jan 22	*ab Initio* Molecular Orbital Theory: From the Beginning
Jan 24	Lab 2: Structure Optimization and Conformational Analysis
Jan 27	Methods for Treating Electron Correlation
Jan 29	Open Shell Systems and Excited States
Jan 31	Lab 3: Thermochemistry in Different QM Model Chemistries
Feb 3	Semi-Empirical MO Methods & Density Functional Theory
Feb 5	Solvation Models for QM Calculations
Feb 7	Lab 4: Tautomeric Preferences and Solvent Effects
Feb 10	Principles of Frontier Orbital Theory
Feb 12	Applications of Frontier Orbital Analysis
Feb 14	Lab 5: Stereoselectivity in Diels-Alder Reactions
Module 2:	**Molecular Mechanics and Dynamics Simulation**
Feb 17	Molecular Mechanics and Force Fields
Feb 19	Advanced Aspects of Force Field Design and Parameterization
Feb 21	Lab 6: Conformational Analysis of Substituted Cycloalkanes
Feb 24	Basics of Molecular Dynamics Simulation
Feb 26	Basics of Monte Carlo Sampling Techniques
Feb 28	Lab 7: Generating and Analyzing a Molecular Dynamics Trajectory **
Mar 3	Methods for Calculation of Free Energy
Mar 5	Application to Intermolecular Interactions & Binding Energies
Mar 7	Lab 8: Calculation of Diffusion Constants from MD
Mar 17	Solvation Models for Use with Empirical Potentials
Mar 19	Hybrid Potentials: Combined QM/MM Simulation
Mar 21	Lab 9: Computing the Hydration Free Energy of Ions
Mar 24	Application of QM/MM to Enzyme Reaction Mechanisms
Mar 26	Prediction of Small Molecular Crystal Structures
Mar 28	Lab 10: Folding of the World's Smallest "Protein"
Module 3:	**Electrostatics, Coarse Graining & Biomolecular Structure Prediction**
Mar 31	Poisson-Boltzmann Equation & Associated Calculations
Apr 2	Application to the Modeling of pKa Values
Apr 4	Lab 11: Running PB Calculations with APBS

Apr 7	Brownian Dynamics Simulations
Apr 9	Coarse Grained Potentials: Tradeoffs & Applications
Apr 11	Lab 12: Work on Individual Student Projects
Apr 14	Useful Tools from Structural Bioinformatics
Apr 16	Critical Assessment of Protein Structure Prediction
Apr 18	Lab 13: Work on Individual Student Projects
Apr 21	Presentation of Student Projects I
Apr 23	Presentation of Student Projects II
Apr 25	Presentation of Student Projects III (if necessary)
May 2	**Final Examination / Projects Due**