

Syllabus

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The course will consist of lectures and hands-on computational labs. There will be one midterm (worth 20%), 5 quizzes (15%), 5 computational assignments (30%), and a major computational project (35%).

Suggested Readings:

"Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian", J. B. Foresman and A. Frisch, 2nd. Ed., Gaussian Inc.

"Molecular Modelling; Principles and Applications", A.R. Leach, 2nd Ed., Prentice Hall.

"Essentials of Computational Chemistry", C.J. Cramer, 2nd Ed., John Wiley and Sons.

"Introduction to Computational Chemistry", F. Jensen, 2nd Ed., John Wiley and Sons.

Tentative Schedule:

Week 1, Jan. 8, 10.

Intro to High Performance Computing (HPC) on the Wayne State Grid.
Population analysis and molecular properties, geometry optimization (Jensen Chs. 9-10)

Week 2, Jan. 15, 17.

Vibrational frequencies, transition states, reaction paths (Cramer Ch. 10, Jensen Chs. 12-13)

Week 3, Jan. 22, 24.

Electron correlation, Density Functional Theory (Cramer Chs. 7-8, Jensen Chs. 4,6)

Week 4, Jan 29, 31.

Model chemistries, thermochemistry (Cramer Ch. 10)

Week 5, Feb. 5, 7.

Molecular Orbital Theory (Cramer Chs. 4-5, Jensen Ch. 3, Leach Ch. 2)

Week 6, Feb. 12, 14.

SCF convergence and stability, excited states (Cramer Ch. 13)

Week 7, Feb. 19, 21.

Assorted special topics in electronic structure theory

Week 8, Feb. 26, 28.

Molecular Mechanics; Empirical Force Fields (Leach Ch. 4, Cramer Ch. 2, Jensen Ch. 2)

Proposals for term projects due

Week 9, Mar. 5, 7.

Classical Simulation Methods (Leach Ch. 6, Cramer Ch. 3, Jensen Ch. 14)

Week 10, Mar. 19, 21.

Molecular Dynamics (Leach Ch. 7, Cramer Ch. 3)

Midterm.

Week 11, Mar. 26, 28.

Monte Carlo (Leach Ch. 8)

Week 12, Apr. 2,4.

Free Energy Perturbation and Solvation (Leach Ch. 11, Cramer Chs. 11-12)

Week 13, Apr. 9, 11.

QM/MM (Cramer Chp. 13)

Week 14, Apr. 16, 18.

Finish working on term projects

Week 15, Apr. 23.

Finals Week

Presentations of term projects