Syllabus

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The course will consist of lectures and hands-on computational labs. There will be one midterm (worth 21%), 5 on-line quizzes (10%), 5 computational assignments (30%), 3 reviews of papers from the scientific literature (9%) and a major computational project (30%).

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.

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

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

Week 1, Jan. 10, 14.

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

Week 2, Jan. 17, 21.

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

Week 3, Jan. 24, 28.

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

Week 4, Jan 31, Feb 4.

Monte Carlo (Leach Ch. 8)

Week 5, Feb. 7, 11.

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

Week 6, Feb. 14, 18.

Population analysis and molecular properties, geometry optimization (Jensen Chs. 9-10)

Week 7, Feb. 21, 25.

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

Week 8, Feb. 28, Mar 4.

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

Proposals for term projects due

Week 9, Mar. 7, 11.

Model chemistries, thermochemistry (Cramer Ch. 10)

Week 10, Mar. 21, 24.

Midterm.

Free Energy Perturbation, Solvation and QM/MM (Cramer Chs. 11-13, Leach Ch. 11)

Week 11, Mar. 28, Apr. 1

MM/QM calculations

Week 12, Apr. 4, 8.

Biochemical Molecular Modeling

Week 13, Apr. 11, 15.

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

Week 14, Apr. 18, 22.

Finish working on term projects

Finals Week

Presentations of term projects