



Week 7, Feb. 20, 24.

Assorted special topics in electronic structure theory

Week 8, Feb. 27, Mar 2.

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

Proposals for term projects due

Week 9, Mar. 5, 9.

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

Week 10, Mar. 19, 23.

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

Midterm.

Week 11, Mar. 26, 30.

Monte Carlo (Leach Ch. 8)

Week 12, Apr. 2,6.

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

Week 13, Apr. 9, 13.

QM/MM (Cramer Chp. 13)

Week 14, Apr. 16, 20.

Finish working on term projects

Finals Week

Presentations of term projects