10.637 (5.697/5.698/10.437): Fall 2016

Quantum Chemical Simulation

Lectures: Tu/Th 11 AM-12:30 PM 4-145 (Labs in 14-0637)

Instructor: Professor Heather J. Kulik
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Course Description: Addresses both the theory and application of first-principles computer simulations methods (i.e., quantum, chemical, or electronic structure), including Hartree-Fock theory, density functional theory, and correlated wavefunction methods. Covers enhanced sampling, ab initio molecular dynamics, and transition-path-finding approaches as well as errors and accuracy in total and free energies. Discusses applications such as the study and prediction of properties of chemical systems, including heterogeneous, molecular, and biological catalysts (enzymes), and physical properties of materials.

Optional source texts for those interested in self-study (specific electronic reading materials will be posted on Stellar in advance of each lecture in most cases).

A Chemist's Guide to Density Functional Theory. Wolfram Koch and Max C. Holthausen

Essentials of Computational Chemistry. Christopher J. Cramer

Both books are available as e-books from the MIT Library System.

Grading:

Homework (four graded labs)	70%
In lab exercises	10%
Journal article presentation	20%

Undergraduates: Homework and exercises only.

Homework: Lab assignments are due two weeks after the in class portion.

Policies: Late homework will be accepted up until the time that solutions are posted but late submissions will be eligible for at most half credit.

10.637 Quantum chemical simulation Fall 2016 Lecture Schedule: *subject to change*

1	Th 9/8	Introduction and overview to the course & getting started with labs
2	Tu 9/13	Molecular mechanics I
3	Th 9/15	*Lab 1: Molecular mechanics*
4	Tu 9/20	Molecular mechanics II
5	Th 9/22	Molecular dynamics
6	Tu 9/27	*Lab 2: Molecular dynamics*
7	Th 9/29	*Lab 2: Molecular dynamics*
8	Tu 10/4	Hartree-Fock theory I and quantum mechanics review
9	Th 10/6	Hartree-Fock theory II
10	Th 10/13	*Lab 3: Hartree-Fock theory*
11	Tu 10/18	Basis sets and effective core potentials
12	Th 10/20	Density functional theory I
13	Tu 10/25	Density functional theory II
14	Th 10/27	*Lab 4: Density functional theory (graded)*
15	Tu 11/01	Special details of periodic DFT
16	Th 11/03	Excited states and time-dependent DFT
17	Tu 11/08	*Lab 5: Excited states with TDDFT*
18	Th 11/10	Post-Hartree-Fock wavefunction theory I
19	Tu 11/15	Perturbation theory
20	Th 11/17	*Lab 6: Correlated wavefunction theory (graded)*
21	Tu 11/22	Post-Hartree-Fock wavefunction theory II
22	Tu 11/29	Ab Initio MD sampling, QM/MM, and environment effects
23	Th 12/01	*Lab 7: QM/MM and environment effects (graded)*
24	Tu 12/06	Advanced density functional theory
25	Th 12/08	*Lab 8: Ab initio MD and advanced modeling*
26	Tu 12/13	Review and Journal presentations

Revised by HJK on 10/13/16