9/8/04

10.675J.5.675J Syllabus (Fall, 2004)
TR 11:00 – 12:30, 66-156

Date	Subject	Assignment Due
Sept. 9	Introduction, textbook & notes, many body Schrödinger equation, density functional theory, examples and inspiration *(computer projector reserved)*	
14, 16	*No class-- Trout on travel*	
21	Electronic spin, spin orbitals, molecular orbital theory, valence bond theory	Review quantum mechanics, Solution of hydrogen atom
23	Hartree-Fock Theory, Matrix manipulations	
28	Mathematical underpinnings, Dirac Notation, G03 calculations	Read SO 1-30
(later) 28	*Electronic Classroom Tutorial, 7:00-8:30 pm in 1-115*	
30	Solution of Hartree-Fock equations, variational principle, mean field theory	PS 1 due
Oct. 5	Solution of H-F equations cont'd, Meaning of eigenvalues, Basis sets intro.	SO 108-122; 131-149
7	Gaussian Basis sets	PS 2 due
12	Correlation, CI, MP perturbation theories	SO 60-64; 320-326; 350-353; study graphs 375-376; skim SO ch.. 4
14	Density functional theory (DFT)- introduction	Read handout on DFT; PS 3 due
19	DFT: solution of Kohn-Sham equations and exchange-correlation functionals	
21	Coupled-Cluster theories, QCISD, G1, G2	skim SO ch. 5; PS 4 due
26	G1, G2 cont'd, comparison, NCSA Teams, projects	Read handouts; Initial choice of project and literature search due
28	The plane-wave pseudopotential method (PWPP)	
Nov. 2	PWPP continued, Introduction to classical molecular	

	dynamics (MD)	
4	Car-Parrinello molecular dynamics- method	
9	*No class- AIChE conference*	
11	*Veteran's Day—Holiday*	
16	Running the Car-Parrinello code	project status report; review molecular dynamics from Nov. 2 and 4 lecture
18	Car-Parrinello molecular dynamics - applications	
23	Embedding, reaction field methods, solvation, Combined QM/MM	PS 5
25	*No Class- Thanksgiving*	
30	Exploring complex free energy landscapes - reactivity	
Dec. 2	Computing reaction rate constants	Project finalized
Sat. 4	*Presentation of projects, 10 a.m. – 1 p.m. in 66-360*	
7	TBD	
9	TBD	

SO: Szabo and Ostlund, **Modern Quantum Chemistry**