Chemistry 4021/8021

Instructor: Laura Gagliardi

Computational Chemistry

Date	Topic
1/22	Introduction, historical perspectives and generalities
	Force Fields / Molecular Mechanics/Huckel MO
1/24	Discussion with respect to the potential energy surface. Discuss videos 02.01 and 02.02
1/27	Problems with respect to the potential energy surface. Discuss videos 02.03-02.05
1/29	Discussion/problems with respect to theory of classical dynamics. Time- and equilibrium-averaged properties. Simulation methods. Discuss videos 02.06-02.08
1/31	Continue discussion/problems with respect to theory of classical dynamics. Time- and equilibrium-averaged properties. Simulation methods. Discuss videos 02.06-02.08
2/3	Discussion/problems with respect to Hückel MO theory. Hartree-Fock theory. MO-LCAO formalism. Videos 03.01-0.3.07 First lab assigned—due 2/21 (HF Theory)
2/5	Continue Discussion/problems with respect to Hückel MO theory. Hartree-Fock theory. MO-LCAO formalism. Videos 03.01-0.3.07
2/7	Discussion of literature application.
	Ab Initio Hartree-Fock Theory
2/10	Catch up
2/12	Visit to the Minnesota Supercomputer Institute. (meet in 125 Walter Library)
2/14	Demo Unix, vi, Gaussian 09 software Interface. Hartree-Fock keywords. Input and Output.
2/17	Hartree-Fock Theory Discussion of Video 04.01
2/19	HF Theory
2/21	First lab due. Discussion of literature application.
2/24	Discussion/problems with respect to theory of HF equations and variational principle. Basis sets. Practical issues. Second lab assigned—due 4/6
2/26	Discussion/problems with respect to **theories** and **applications** specific to hypersurface construction. Closed shell and open-shell molecules. One-electron properties.

	Density Functional Theory
2/28	DFT 1 Videos 05.01 to 05.08
3/2	DFT 2 Discussion/problems with respect to Kohn-Sham theory with historical context. Modern functionals. Basis sets. Compare and contrast with HF techniques. Current frontiers. Software.
3/4	DFT 3 Discussion of literature application.
3/6	Catch up
3/9	Spring Break
3/11	Spring Break
3/13	Spring Break
3/16	Catch Up and DFT literature discussion
3/18	Catch Up
3/20	MIDTERM EXAM I
	Electron Correlation beyond HF
3/23	Beyond HF Video 04.02-04.03
fy3/25	Multireference methods
3/27	Dynamic correlation
3/30	Multiconfiguration pair-density functional theory
4/1	Literature discussion on electron correlation
4/3	Catch Up
4/6	Second lab due. Discussion/problems with respect to theories and applications specific to various spectroscopies and thermodynamics. Discuss second lab. Video 04.04
	Periodic Systems
4/8	Periodic Solids and Band Structure Theory.
4/10	One-electron properties, Defect, and Chemist's perspective.
4/13	Review and Examples on calculating semiconducting band gap and defect.
4/15	Catch up and review
4/17	MIDTERM EXAM II
	Condensed-phase Calculations Implicit/Explicit Solvation Models
4/20	Third lab assigned—due 5/1. MIDTERM EXAM II

4/22	Discussion/problems with respect to condensed phase effects in general. Thermodynamic and kinetic effects. Poisson-Boltzmann equation—theory and implementation
4/24	Discussion/problems with respect to explicit solvent models. Monte Carlo and Molecular Dynamics.
4/27	Discussion/problems with respect to theory of hybrid quantum mechanics/molecular mechanics methods (QM/MM).
4/29	Discussion of literature application. (Haranczyk et al. J Chem Inf Model 52 (2012) 2902)
5/1	Third lab due. Discuss third lab.
5/4	Machine Learning literature discussion
5/6	Machine Learning literature discussion
5/8	Discussion and Catch Up

5/15 (1:30–3:30 PM)

Final Exam *and Paper Analysis Due (8021 only)*