

# Chemistry 4021/8021

## *Computational Chemistry*

Date

### 1/22 I. Introduction and Historical Perspectives and Generalities

### II. Force Fields / Molecular Mechanics

*Reading: Cramer, Chapters 1-3. Online videos: (II.i–viii)*

1/24 A. Discussion/problems with respect to the Potential Energy Surface.

1/27 No class scheduled. 101D Smith open.

1/29 B. Discussion/problems with respect to **theory** of classical mechanics. Parametrization of force fields. Bonded and non-bonded terms. MM2, MM3, OPLS, etc. Geometry optimization. Computer implementations — hardware and software.

1/31 C. **Demo** PC Model (meet in 101D Smith Hall).

2/3 D. Discussion/problems with respect to **theory** of classical dynamics. Time- and equilibrium-averaged properties. Simulation methods. *First lab assigned—due 2/26*

2/5 E. Discussion of literature **application**. (Nicholas et al. J Am Chem Soc 113 (1991) 4792 -- all literature assignments may be downloaded from <http://www.lib.umn.edu/walter/collections> (follow the Chemistry e-Journals link))

2/7 No class scheduled. 101D Smith open.

### III. Semiempirical Theory

*Reading: Cramer, Chapters 4 and 5.  
([http://www.gaussian.com/g\\_tech/1.htm](http://www.gaussian.com/g_tech/1.htm)) Online videos: (III.i–vii)*

2/10 No class scheduled. 101D Smith open.

2/12 A. Discussion/problems with respect to Hückel MO **theory**. Hartree-Fock **theory**. MO-LCAO formalism. (*CJC attends via Skype*)

2/14 B. Visit to the Minnesota Supercomputer Institute. (meet in 125 Walter Library -- MSI guest lecturers Ben Lynch and Nancy Rowe).

2/17 No class scheduled. 101D Smith open.

- 2/19 C. Discussion/problems with respect to CNDO, INDO and NDDO approximations. Parameterization of semiempirical terms. Survey of modern Hamiltonians (AM1, PM3, MNDO/d, PM6, OM1, PDDG, etc.)
- 2/21 D. Discussion of literature **application**. (Anders et al. J Comp Chem 14 (1993) 1301)
- 2/24 No class scheduled. 101D Smith open.
- 2/26 E. **First lab due**. Discussion of literature **application**. (Kozlowski et al. J Am Chem Soc 125 (2003) 6614 and Ianni et al. Angew Chem Intl Ed 45 (2006) 5502) *Discuss first lab*.
- 2/28 F. **Demo** Unix, vi, Gaussian 09 **software** (meet in 101D Smith). Interface. Semiempirical keywords. Input and Output.

#### IV. Ab Initio Hartree-Fock Theory

*Reading: Cramer, Chapters 6, 7, 9, and 10. Gaussian 09 manual ([http://www.gaussian.com/g\\_tech/1.htm](http://www.gaussian.com/g_tech/1.htm)). Online videos: (IV.i–viii)*

- 3/3 No class scheduled. 101D Smith open.
- 3/5 A. Discussion/problems with respect to **theory** of HF equations and variational principle. Basis sets. Practical issues. **Second lab assigned—due 4/7**
- 3/7 B. Discussion/problems with respect to **theory** of electron correlation techniques and implementation.
- 3/10 No class scheduled. 101D Smith open.
- 3/12 C. Discussion/problems with respect to **theories** and **applications** specific to hypersurface construction. Closed shell and open-shell molecules. One-electron properties.
- 3/14 **MIDTERM EXAM I**

#### V. Density Functional Theory

*Reading: Cramer, Chapter 8, 9, and 10. Gaussian 09 manual ([http://www.gaussian.com/g\\_tech/1.htm](http://www.gaussian.com/g_tech/1.htm)). Online videos: (V.i–viii)*

- 3/24 No class scheduled. 101D Smith open.

- 3/26–3/28 B. Discussion/problems with respect to Kohn-Sham **theory** with historical context. X- $\alpha$ . Modern functionals. Basis sets. Compare and contrast with HF techniques. Current frontiers. **Software**.
- 3/31 No class scheduled. 101D Smith open.
- 4/2 C. Discussion of literature **application**. (Lewin and Cramer Molecular Pharmaceutics 1 (2004) 128)
- 4/4 D. Discussion of literature **application**. (Sillar and Sauer J Am Chem Soc 134 (2012) 18354)
- 4/7 E. **Second lab due**. Discussion/problems with respect to **theories** and **applications** specific to various spectroscopies and thermodynamics. *Discuss second lab.*
- 4/9 **MIDTERM EXAM II**
- 4/11 No class scheduled. 101D Smith open.

## VI. Condensed-phase Calculations

*Reading: Cramer, Chapters 11 and 12. Gaussian 09 manual ([http://www.gaussian.com/g\\_tech/1.htm](http://www.gaussian.com/g_tech/1.htm)). Online videos: (VI.i–vii)*

- 4/14 No class scheduled. 101D Smith open.
- 4/16 A. Discussion/problems with respect to condensed phase effects in general. Thermodynamic and kinetic effects. Poisson-Boltzmann equation—**theory** and implementation. **Third lab assigned—due 5/7**.
- 4/18 B. Discussion/problems with respect to continuum solvent models. Kirkwood-Onsager and more general models. **Selection of 8021 paper for critical analysis due**.
- 4/21 No class scheduled. 101D Smith open.
- 4/23 C. Discussion/problems with respect to explicit solvent models. Monte Carlo and Molecular Dynamics.
- 4/25 D. Discussion of literature **application**. (Wood et al. J Chem Theor Comput 4 (2008) 1788)

## VII. Advanced Topics

*Reading: Cramer, Chapters 13, 14, and 15. Online videos: (VII.i–x)*

- 4/28 No class scheduled. 101D Smith open.
- 4/30 A. Discussion/problems with respect to **theory** of hybrid quantum mechanics/molecular mechanics methods (QM/MM).
- 5/2 B. Discussion of literature **application**. (Haranczyk et al. J Chem Inf Model 52 (2012) 2902)
- 5/5 C. Discussion/problems with respect to **theory** for dealing with excited states and non-single-determinantal states.
- 5/7 D. **Third lab due**. Discussion/problems with respect to **theory** of gas-phase reaction dynamics. *Discuss third lab*.
- 5/9 No class scheduled. 101D Smith open.
- 5/15 (1:30–3:30 PM)  
**Final Exam and Paper Analysis Due (8021 only)**