

Chemistry 4021/8021

Computational Chemistry

Date

1/21 **I. Introduction and Historical Perspectives and Generalities**

II. Force Fields / Molecular Mechanics

Reading: Cramer, Chapters 1-3.

1/23–1/26 A. **Theory** of classical mechanics. Parametrization of force fields. Bonded and non-bonded terms. MM2, MM3, OPLS, etc. Geometry optimization. Computer implementations — hardware and software.

1/28 B. **Theory** of classical dynamics. Time- and equilibrium-averaged properties. Simulation methods.

1/30 C. **Demo** PC Model (meet in 101D Smith Hall).

2/02 D. Discussion of literature **application**. (Nicholas et al. J Am Chem Soc 113 (1991) 4792 -- all literature assignments may be downloaded from <http://sciweb.lib.umn.edu/ej/ChCEMS.phtml>)

2/04 E. Discussion of literature **application**. (Koska et al. J Chem Inf Model 48 (2008) 1965) *First lab assigned—due 2/23.*

III. Semiempirical Theory

Reading: Cramer, Chapters 4 and 5.

2/06–2/11 A. Hückel MO **theory**. Hartree-Fock **theory**. MO-LCAO formalism. CNDO, INDO and NDDO approximations. Parameterization of semiempirical terms. Survey of modern Hamiltonians (AM1, PM3, MNDO/d, PM6, OM1, PDDG, etc.)

2/13 B. General performance of modern semiempirical models. Use in SAR and SAR-like processes.

2/16 C. Molecular geometry representation. Z-matrices. Symmetry.

2/18 D. **Demo** Chem-3D **software** (meet in 101D Smith). Interface. Input and Output.

2/20* E. Discussion of literature **application**. (Anders et al. J Comp Chem 14 (1993) 1301)

2/23* F. *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.*

IV. Ab Initio Hartree-Fock Theory

Reading: Cramer, Chapters 6, 7, 9, and 10. Gaussian03 manual (www.gaussian.com/g_ur/g03mantop.htm).

- 2/25–3/02 A. Review **theory** of HF equations and variational principle. Basis sets. Practical issues. Electron correlation techniques and implementation. **Applications.** Hypersurface construction. Closed shell and open-shell molecules. One-electron properties.
- 3/04–3/06 B. **Theories** and **applications** specific to various spectroscopies and thermodynamics.
- 3/09 C. Serious computers. Memory and Disk. General discussion of the interdependence of computational **software** and **hardware**. Tour of MSI machine room (meet in 402 Walter Library -- MSI lecture room -- Dr. Ben Lynch guest lecturer).
- 3/11 C. **Demo** Unix, vi, Gaussian 03 (meet in 101D Smith). Keywords, input and output. *Second lab assigned—due 4/06.*
- 3/13 **MIDTERM EXAM**

V. Density Functional Theory

Reading: Cramer, Chapter 8, 9, and 10. Gaussian03 manual (www.gaussian.com/g_ur/g03mantop.htm).

- 3/23–3/25 A. Derive Kohn-Sham **theory** with historical context. X- α . Modern functionals. Basis sets. Compare and contrast with HF techniques. Current frontiers. **Software**.
- 3/27* B. Discussion of literature **application**. (Ahlquist et al. Organometallics 25 (2006) 2066)
- 3/30* C. Discussion of literature **application**. (Sander et al. Chem Eur J 14 (2008) 9714)
- 4/01* D. Discussion of literature **application**. (Lewin and Cramer Molecular Pharmaceutics 1 (2004) 128)

VI. Condensed-phase Calculations

Reading: Cramer, Chapters 11 and 12. Gaussian03 manual (www.gaussian.com/g_ur/g03mantop.htm).

- 4/03 A. Condensed phase effects in general. Thermodynamic and kinetic effects. Poisson-Boltzmann equation—**theory** and implementation.
- 4/06 B. *Second lab due.* Continuum solvent models. Kirkwood-Onsager and more general models. *Discuss second lab.*

- 4/08 C. Explicit solvent models. Monte Carlo and Molecular Dynamics. **Software.**
- 4/10* D. Discussion of literature **application.** (Cramer and Truhlar J Am Chem Soc 115 (1993) 8810) *Third lab assigned—due 5/04.*
- 4/13* E. Discussion of literature **application.** (Nagan et al. J Am Chem Soc 121 (1999) 7310)
- 4/15* F. Discussion of literature **application.** (Wood et al. J Chem Theor Comput 4 (2008) 1788)

VII. Advanced Topics

Reading: Cramer, Chapters 13, 14, and 15. Gaussian03 manual (www.gaussian.com/g_ur/g03mantop.htm).

- 4/17 A. **Theory** of hybrid quantum mechanics/molecular mechanics methods (QM/MM).
- 4/20* B. Discussion of literature **application.** (Cramer and Pak Theor Chem Acc 105 (2001) 477)
- 4/22* C. Discussion of literature **application.** (Tuttle et al. J Phys Chem B 111 (2007) 8321)
- 4/24-4/27 D. **Theory** for dealing with excited states and non-single-determinantal states. *Selection of 8021 paper for critical analysis due 4/24.*
- 4/29* E. Discussion of literature **application.** (Orlova et al. J Am Chem Soc 125 (2003) 6962)
- 5/01* F. Discussion of literature **application.** (Puzyn et al. J. Chem Inf Model 48 (2008) 1174)
- 5/04* G. *Third lab due.* Discussion of literature **application.** (Nam et al. J Am Chem Soc 130 (2008) 4680) *Discuss third lab. Final exam distributed.*
- 5/06 H. **Theory** of gas-phase reaction dynamics.
- 5/08* I. Discussion of literature **application.** (Woodrum and Cramer Organometallics 25 (2006) 68)
- 5/15 **Final Exam Due and Paper Analysis (8021 only)**

* A quiz is possible on this date.