Computational Chemistry

Chemistry 4021/8021, Spring Semester 2022

Instructor: Jiali Gao, 241A Smith Hall, 625-0769, jgao@umn.edu.
TA: Not available this semester (000)
Time: Lectures: M.W.F.: 9:05 – 9:55 am,
Canvas online lectures and practices.

Office Hours: JG, 1-3 pm on Wednesday online via zoom (link from canvas)

Text (reference only):
A technical and practical reference:

1. James B. Foresman and Aeleen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc. $35 including shipping, see: https://gaussian.com/expchem3/

Reference on topics:

2. Christopher J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2nd Ed. Wiley & Sons, New York.
3. Andrew R. Leach, Molecular Modelling: Principles and Applications, 2nd Ed., Prentice Hall, 2001.
4. Frank Jensen, Introduction to Computational Chemistry, Wiley, 2nd Ed., 2007.

In addition, I will make extensive use of "handouts", covering major topics to be discussed in class, which will be posted on the class Moodle site.

The Course: This is a project-oriented course, and team efforts are encourage.

- We will be working on a set of 10 projects.
  Each project will contain a number of problems, and the main purpose is to provide you a practical understanding of computation, through which further insights can be gained on structure and properties of molecules.
- I will randomly select 5 projects for grading.
  These assignments should be turned in on time, or it will not be graded until the end of the semester. You can work individually, but you are strongly encouraged to work and discuss the projects together to accomplish the goals of the projects. However, you will need to write your own summary and project reports.
- Two main software packages: Gaussian16 for quantum chemistry and CHARMM for molecular dynamics of condensed-phase and biological systems.
  I will typically emphasize the practical use of these programs, and discuss key background materials in classes. However, the mathematical and algorithmic details will be limited to the minimal amount. My intension is to provide you with the basic background of computational chemistry, and the essential skills to do computation. You need to learn the necessary hardware and software introduced in the class.

Requirements:

- Your efforts.
- Basic quantum mechanics and statistical thermodynamics (Chem4501 and 4502).
- Access to a laptop or a computer during class hours.
- Basic knowledge of Unix operating system, HPC access, and a file editor (vi).

See, https://www.msi.umn.edu/sites/default/files/unix2013.6.18.pdf.

Computer Accounts and Software: A computer account has been assigned to each of you (who registered two weeks before classes start), and an email from the Minnesota Supercomputing Institute (MSI) has been sent to you with login information. Your local computer will be connected to the HPC computers at MSI via Wifi.

Computational chemistry and modeling packages:

(1). Gaussian (electronic structure)
(2). CHARMM (statistical mechanical simulation and modeling)

Visualization software:

(3). GaussView (GUI to Gaussian)
(4). CHARMM-GUI (GUI for CHARMM input, see http://www.charmm-gui.org/)
(5). VMD (for molecular graphics visualization, especially macromolecules).
(6). Molden (molecular graphics, http://www.cmbi.ru.nl/molden/molden.html).

Grading: Your final grade will be determined based on the following:

- homework assignments (60 pts)
- one mid-term exam (20 pts) on March 16.
- the final exam/project (20 pts).

Homework and exam projects will be evaluated on the ***correctness*** of your work, ***thoroughness*** of data and analysis, ***clarity*** in writing, and ***professionalism*** in presentation.

Incomplete: Will be given only under exceptional circumstances, such as an extended illness certified by a medical doctor, and Department policies dictate that you must have a passing grade on all midterm exams and only miss the final exam. If you receive an incomplete, you must complete all requirements to remove the incomplete by the end of the following academic year, i.e., the Spring semester, 2023, or the incomplete will automatically be changed to an F.

Missed Exam/projects: Any unexcused absence from an examination or failed to turn in homework assignment will result in a grade of zero points for that exam or homework. You should get permission before the exam if you must be absent from an exam. Personal business will not be accepted as an excuse, so, you should make plan of your schedule accordingly.

Policy on Academic Dishonesty: Please visit the Office for Student Conduct and Academic Integrity: http://www.oscai.umn.edu/conduct/student/index.html.
Additional information on a range of 11 policies may be found at https://policy.umn.edu/education/syllabusrequirements-appa.

Course Outline

(Dates are tentative)

Date	Topic	Reading (Cramer, FF:Foresman, Frisch)
Introduction to HPC, operating systems, software, and access.		
1/19	Introduction	2.2, Chpt. 4
1/21	HPC and access, Unix OS, vi editor, and software	notes, & unix tutorials
Potential energy surface		
1/24	Prob. 1, strain energies	
	Gaussian and GaussView, PES	FF
1/26	Minimization techniques (I)	2.4 & hand-outs
1/28	Orbitals, basis sets, determinant, and SCF	6.1-3
Intermolecular interactions		
1/31	Prob. 2: hydrogen bond and vdW forces	
2/2	Intermolecular forces	
3/4	Hartree-Fock theory	6.4
Molecular properties		
2/7	Prob. 3: IP, EA, dipole moment, IR	
2/9	Bonding and orbital interactions	Hoffmann
2/11	Kohn-Sham density functional theory	Chpt. 8
Thermochemistry		
2/14	Prob. 3: PA, GB, ΔH_f, BDE	Chpt. 10
2/16	TS optimization (II), chemical kinetics	2.4 & hand-outs
2/18	Free radicals, electronic spin, open shell	15.1-3
Reaction mechanisms		
2/21	Prob. 4: PES scan, ΔH_{rxn}, $\Delta G^{\neq}$ for n1, Sn2, E1, E2	
2/23	IRC, Reaction path following	
2/25	Why cannot I dissociate a chemical bond?!	
Chemical accuracy		
2/28	Prob. 5: TS optimizations and PES	7.1, 7.4
3/2	MP2, CI, MCSCF, and the golden standard	7.1-6
3/4	Static vs. dynamic correlation	7.2-6
3/7-11	**Spring break**	
Solvation (I)		
3/14	Prob. 6: acetone, pyridine and pyrimidine, Continuum solvation models	

Mid-term exam: Date March 16.

3/18	equilibrium and nonequilibrium solvation	

Excited states

3/21	Prob. 6: absorption and emission, ECD, NH_3 dissociation	
3/23	CI, CASPT2, EOM-CCSD	
3/25	TD-DFT	

Molecular dynamics

3/28	Prob. 7: liquid water	Chpt. 3
3/30	Force fields, Stat-mech. simulation techniques	2.2-3
4/1	RDF, diffusion, and visualization; VMD	

Free energy

4/4	Prob. 8: keto-enol equil., ΔpKa and pKa	12.1-3
4/6	QM/MM, and FEP	
4/8	Enhanced sampling	

Combined QM/MM (solvation II)

4/11	Prob. 9: PMF for decarboxylation and S_N2 rxns
4/13	Umbrella sampling
4/15	Dual-level models to achieve accuracy

Proteins and enzymes

4/18	Prob. 10: Protein MD
4/20	Protein structure and dynamics
4/22	Protein-ligand interactions

Proteins and enzymes

4/25	Prob. 10: Enzyme/protein-inhibitor interactions Optional: polarization of inhibitor in the active site
4/27	QM/MM energy decomposition analysis
4/29	X-Pol: a next-generation force field

Review

5/2	Review of Computational Chemistry

Final Exam Project: May 2-11.