COMPUTATIONAL QUANTUM CHEMISTRY
CHM 673, Spring 2020

Course Description
This course aims to give the students both theoretical and practical background in the computational techniques used in modern quantum chemistry. A significant fraction of the students' time will be spent actually using quantum chemistry programs. The last assignment will provide a chance for students to perform an independent computational project related to their research interests and present a seminar to the class. A solid undergraduate background in Physical Chemistry or, preferably, Quantum Mechanics, will suffice as a prerequisite.

Topics Covered
- Preliminaries: central approximations and important concepts in molecular modeling
- Self-consistent field theory
- Density functional theory
- Potential energy surfaces and chemical reactions
- Achieving chemical accuracy
- Electronically excited and open-shell species
- Introduction to modeling chemistry of extended systems

Instructor: Prof. Lyudmila Slipchenko, WTHR 265H, lslipchenko@purdue.edu
office hours: W 1:30-2:30 pm

Classes
T,Th 12:00-1:15 pm, BRWN 3102

Course materials
https://github.com/slipchenko/CHM673

RCAC Scholar server at /depot/lslipche-class

Grading
Lab and homework assignments: 40%
Midterm: 20%
Project: 30%
Tuesday quizzes and class participation: 10%
Homework, lab, and project assignments are announced on Thursdays and are due on next Tuesdays (in 12 days).

Textbooks
Required
- F. Jensen, *Introduction to Computational Chemistry*, (Wiley, New York, 2017)
- A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st ed., revised (Dover, 1996)
Optional
- J. Schrier, *Introduction to Computational Physical Chemistry*, (University Science Books, 2017)

Material coverage

1. Schrodinger equation. Review of QM. Born-Oppenheimer approximation.
Relevant reading: Review of elementary linear algebra: chapter 1 from S&O.
Electronic problem and BO approximation: http://vergil.chemistry.gatech.edu/notes/bo/bo.html; chapter 3.1 from Jensen; chapter 2.1 from S&O.

2. Chemical reactions and potential energy surfaces.
Relevant reading: geometry optimization: chapters 13.1-13.4 from Jensen;
Vibrational normal coordinates: chapter 17.2.2 from Jensen;
Chemical reactions: chapter 13.8 from Jensen
Q-Chem webinar: https://www.youtube.com/watch?v=JBBblxGEXxo&feature=youtu.be

3. Orbitals and Slater determinants. Theoretical model chemistries.
Relevant reading: Chapter 2.2 (pg. 46-64) from S&O;
http://vergil.chemistry.gatech.edu/notes/hf-intro/hf-intro.html

4. Hartree-Fock theory. Koopmans' theorem.
Relevant reading: Chapter 3.1, 3.2 from S&O; chapters 3.2-3.4, 3.8 from Jensen;
http://vergil.chemistry.gatech.edu/notes/hf-intro/hf-intro.html;
http://vergil.chemistry.gatech.edu/notes/permsymm/permsymm.html;

5. Basis sets.
Relevant reading: chapter 3.3, 3.4, 3.6 from S&O; 3.5, 5.1-5.4 from Jensen;

6. Molecular orbitals. Point group symmetry.
Relevant reading:
http://vergil.chemistry.gatech.edu/notes/grpthy-vib/grpthy-vib.html

7. Spin operators. Restricted and unrestricted HF.
Relevant reading: Spin operators: chapter 2.5 from S&O.
RHF and UHF: chapter 2.5 from S&O. H_2 dissociation: chapter 3.8.7 from S&O; chapters 3.7, 4.3-4.4 from Jensen.

8. Density functional theory.
Relevant reading:
Chapters 6.1,6.2, 6.5-6.8, 6.11-6.12 from Jensen;
Q-Chem webinar: https://www.youtube.com/watch?v=C5iiivjIn58
ICTS talk: https://www.youtube.com/watch?v=AoQmb4Vz24U

9. Electron correlation. Configuration interaction. Size-consistency problem. Wave function versus electron density approaches.
Relevant reading:
electron correlation: chapters 2.2.6-2.2.7 from S&O; chapter 4.1 from Jensen;
CI: http://vergil.chemistry.gatech.edu/notes/ci/ci.html; chapters 4.2, 4.5 from Jensen; chapters 4.1, 4.2, 4.6 from Szabo

10. Dynamical correlation. Second-order perturbation theory. Coupled cluster theory. Extrapolation techniques. Performance of electronic structure methods.
Relevant reading:
MP2: chapters 6.1, 6.5 from S&O, chapter 4.8 from Jensen.
Coupled cluster theory: chapters 4.9-4.10 from Jensen
Extrapolation techniques: chapters 5.9, 5.10 from Jensen
Performance of electronic structure methods: 4.13, 12.1-12.6 from Jensen

11. Non-dynamical correlation. Multi-configuration SCF.
Relevant reading:
MCSCF: chapters 4.6, 4.7 from Jensen, chapter 4.5 from S&O

12. Electronic excited states. CIS, TD-DFT, EOM-CCSD
Relevant reading:
Excited states: chapter 4.14 from Jensen
EOM-CC: Q-Chem webinar:
https://www.youtube.com/watch?v=Adf_F6IatrU&feature=youtu.be
TD-DFT: chapter 6.9 from Jensen

13. Chemistry of extended and periodic systems: solvation models, QM/MM, fragmentation methods, periodic DFT
Relevant reading:
Chapters 2.12, 4.12 from Jensen

Purdue Honors Pledge

The following pledge has been written by Purdue students:
"As a boilermaker pursuing academic excellence, I pledge to be honest and true in all that I do. Accountable together - we are Purdue." See
https://www.purdue.edu/provost/teachinglearning/honor-pledge.html

Student Well-Being
CAPS Information: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of support, services are available. For help, contact Counseling and Psychological Services (CAPS) at (765)494-6995 and http://www.purdue.edu/caps/ during and after hours, on weekends and holidays, or by talking directly to a counselor in the Purdue University Student Health Center (PUSH) during business hours.

EMERGENCY RESPONSE PROCEDURES:
Review the **Emergency Procedures Guidelines**
https://www.purdue.edu/emergency_preparedness/flipchart/index.html
Review the **Building Emergency Plan** (available on the Emergency Preparedness website or from the building deputy) for:

- evacuation routes, exit points, and emergency assembly area
- when and how to evacuate the building.
- shelter in place procedures and locations
- additional building specific procedures and requirements.

EMERGENCY PREPAREDNESS AWARENESS VIDEOS
Run. Hide. Fight.® is a 6-minute active shooter awareness video that illustrates what to look for and how to prepare and react to this type of incident. See:
https://www.youtube.com/watch?v=5mzI_5aj4Vs (Link is also located on the EP website)

MORE INFORMATION
Reference the Emergency Preparedness web site for additional information:
https://www.purdue.edu/ehps/emergency_preparedness/

EMERGENCY NOTIFICATION PROCEDURES are based on a simple concept – if you hear a fire alarm inside, proceed outside. If you hear a siren outside, proceed inside. To report an emergency call 911.

• **Indoor Fire Alarms** mean to stop class or research and immediately **evacuate** the building. o Proceed to your Emergency Assembly Area away from building doors. **Remain outside** until police, fire, or other emergency response personnel provide additional guidance or tell you it is safe to leave.

• **All Hazards Outdoor Emergency Warning Sirens** mean to immediately seek shelter (**Shelter in Place**) in a safe location within the closest building. o "Shelter in place" means seeking immediate shelter inside a building or University residence. This course of action may need to be taken during a tornado, an active threat including a shooting or release of hazardous

materials in the outside air. Once safely inside, find out more details about the emergency.** **Remain in place** until police, fire, or other emergency response personnel provide additional guidance or tell you it is safe to leave.

*** Seek additional clarifying information by all means possible…Purdue Emergency Status page, text message, Twitter, Desktop Alert, Albertus Beacon, digital signs, email alert, TV, radio, etc.…review the Purdue Emergency Warning Notification System multi-communication layers at http://www.purdue.edu/ehps/emergency_preparedness/warning-system.html*