**COMPUTATIONAL QUANTUM CHEMISTRY**
**CHM 673, Spring 2024**

**Instructor:** Prof. Lyudmila Slipchenko, WTHR 265H, lslipchenko@purdue.edu

**Classes**
T,Th 10:30-11:45 am, BRWN 3100

**Office hours**
Tue 12:00-1:00 pm & by appointment, WTHR 265H

**Course materials**
Brightspace course page https://purdue.brightspace.com/d2l/le/content/947312/Home
Github page with course resources https://github.com/slipchenko/CHM673

**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)

**Grading**
Computational lab and homework assignments: 40%
Midterm: 20%
Project: 30%
Weekly quizzes and class participation: 10%

**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.

**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. 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.

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

8. 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

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

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. 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

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

**Quarantined/isolated students**
If you become quarantined or isolated at any point in time during the semester, in addition to support from the Protect Purdue Health Center, you will also have access to an Academic Case Manager who can provide you academic support during this time. Your Academic Case Manager can be reached at acmq@purdue.edu and will provide you with general guidelines/resources around communicating with your instructors, be available for academic support, and offer suggestions for how to be successful when learning remotely. Importantly, if you find yourself too sick to progress in the course, notify your academic case manager and notify me via email or Brightspace. We will make arrangements based on your particular situation. The Office of the Dean of Students (odos@purdue.edu) is also available to support you should this situation occur.

**Course schedule**
The material covered in the course is presented under Material Coverage section (see below), lecture notes will be posted on the Brightspace web page. Depending on student content of the current class some of the additional topics will be included (TBA).

**Attendance policy**
Students should stay home and contact the Protect Purdue Health Center (496-INFO) if they feel ill, have any symptoms associated with COVID-19, or suspect they have been exposed to the virus. In the current context of COVID-19, in-person attendance will not be a factor in the final grades, but the student still needs to inform the instructor of any conflict that can be anticipated and will affect the submission of an assignment or the ability to take an exam. Only the instructor can excuse a student from a course requirement or responsibility. When conflicts can be anticipated, such as for many University-sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible. For unanticipated or emergency conflict, when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, through Brightspace, or by phone. When the student is unable to make direct contact with the instructor and is unable to leave word with the instructor's department because of circumstances beyond the student's control, and in cases of bereavement, quarantine, or isolation, the student or the student's representative should contact the Office of the Dean of Students via email or phone at 765-494-1747. Our course Brightspace includes a link on Attendance and Grief Absence policies under the University Policies menu.

**Academic Integrity.**
Academic integrity is one of the highest values that Purdue University holds. Individuals are encouraged to alert university officials to potential breaches of this value by either emailing integrity@purdue.edu or by calling 765-494-8778. While information may be submitted anonymously, the more information is submitted the greater the opportunity for the university to investigate the concern. More details are available on our course Brightspace table of contents, under University Policies.

**Nondiscrimination Statement**
Purdue University is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, the University seeks to develop and

nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life. More details are available on our course Brightspace table of contents, under University Policies.

**Accessibility**
Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: drc@purdue.edu or by phone: 765-494-1247. More details are available on our course Brightspace under Accessibility Information.

**Mental Health Statement**
If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try WellTrack. Sign in and find information and tools at your fingertips, available to you at any time.

If you need support and information about options and resources, please contact or see the Office of the Dean of Students. Call 765-494-1747. Hours of operation are M-F, 8 am- 5 pm.

If you find yourself struggling to find a healthy balance between academics, social life, stress, etc. sign up for free one-on-one virtual or in-person sessions with a Purdue Wellness Coach at RecWell. Student coaches can help you navigate through barriers and challenges toward your goals throughout the semester. Sign up is completely free and can be done on BoilerConnect. If you have any questions, please contact Purdue Wellness at evans240@purdue.edu.

If you're struggling and need mental health services: 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 mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at 765-494-6995 during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

**Emergency Preparation**
In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.