Chem 515: Computational Chemistry, Fall 2024

Instructor: Yuezhi Mao (he/him/his)
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Office location: GMCS 213D
Lecture meetings: Tuesday, Thursday 5:00-6:15pm, GMCS-245 (note: this class is in-person)
Practice sessions: Same time and location as lecture
Office hours: Tuesday 3-4 PM, and Thursday 10:30-11:30am
Office hours are *hybrid*; Zoom link: https://SDSU.zoom.us/j/84372262900
Prerequisite: Credit or concurrent registration in CHEM 410B, or graduate standing; knowledge of undergraduate-level quantum chemistry (CHEM 410A or equivalent) is expected

General Information:
This course will provide a broad survey of the field of computational chemistry focusing on (i) *electronic structure theory* (or *quantum chemistry*, a term often used interchangeably) and (ii) *molecular dynamics (MD) simulations*. The advances in chemical theory based on the principles of quantum mechanics and statistical mechanics as well as the development of computational algorithms and software tools have revolutionized the way how researchers approach chemistry, making chemistry no longer a pure experimental science. When used properly and interpreted correctly, computations can provide unprecedented microscopic insights into mechanisms of a broad range of chemical phenomena and processes, including but not limited to chemical reactions in the gas and condensed phases, absorption and emission of light by molecules and materials, and the action of small-molecule drugs on specific sites of biomolecules. In other word, these computations constitute *numerical experiments* whose conditions are controlled by the user through the input file by specifying the relevant parameters such as the molecular structure, temperature/pressure, solvent environment, etc. Such an "experiment" will then be conducted within a given level of theory by executing a computer program, and the results will be produced in the form of computational output files, which need to be further processed by the user to extract the specific information regarding a chemical system or a dynamical process of interest.

While it might be easy to download a computational chemistry program and start running a few calculations following tutorials, it requires knowledge and skills to ensure that the calculations can finish in a reasonable amount of time and provide reasonably accurate results. There are common pitfalls that one should try their best to avoid. Our course will cover both the *fundamental principles* and *practical aspects* of the computational methods introduced. Besides *lectures*, there will be *practice sessions* (computer labs) in which the students will gain hands-on experience on preparing and running calculations and analyzing the results. The graduate students are also required to complete a *mini computational project*, through which they will further practice the knowledge and skills they learned in this class and connect them to their own research.

Student Learning Objectives:

At the end of this course, the student will be able to:

- Articulate what state-of-the-art computational chemistry can achieve and how computations/simulations can benefit their own research
- Explain the basic ideas underlying the modern electronic structure methods covered in this course and the strengths and weaknesses of each method
- Select an appropriate level of electronic structure theory for a given system, choose the correct job type for a specific task, and incorporate environment effects in electronic structure calculations for practical systems
- Set up Q-Chem calculations to predict energies, molecular structures, reactivities, noncovalent interactions, and various types of spectra (UV-Vis, IR, etc.); execute Q-Chem (and other software packages) on a Linux server/cluster; use analysis and visualization tools to interpret the results of quantum chemistry calculations
- Explain the basic principles and practical aspects of molecular dynamics (MD) simulations; prepare MD simulations for molecules in the solution phase and large biomolecules; compute static and dynamical properties from MD trajectories obtained
- Interpret, discuss, and evaluate journal articles reporting a full computational study of a given chemical problem or the investigation of a series of chemical systems; extract useful information regarding how to select computational methods from benchmark studies of computational methods
- Recognize and provide examples for the essential role of diversity, equity, and inclusion in the progression of the field of computational chemistry

Tentative course calendar:

Date	Content	Note
08/27 (Tu)	Course info; introduction to computational chemistry	
08/29 (Th)	Quantum mechanics recap; variational method	
09/03 (Tu)	Born-Oppenheimer Approximation; electronic Hamiltonian; many-electron wavefunctions	
09/05 (Th)	Hartree-Fock theory and self-consistent field (SCF) calculations	
09/10 (Tu)	Hartree-Fock wrap-up; introduction to IQmol	
09/12 (Th)	Atomic basis sets in quantum chemistry	
09/17 (Tu)	Practice 1: Building molecules using IQmol; Hartree-Fock energy calculations; basis set convergence	
09/19 (Th)	Basis sets (cont'd) and effective core potentials; fundamentals of density functional theory (DFT)	In-class Quiz 1
09/24 (Tu)	The Kohn-Sham formalism; "Jacob's ladder" for density functionals; dispersion corrections in DFT	Practice 1 report due
09/26 (Th)	DFT benchmarks, practical aspects, and caveats	
10/01 (Tu)	Practice 2: DFT calculations using Q-Chem	

10/03 (Th)	Geometry optimization and harmonic frequency calculations	
10/08 (Tu)	Transition state search; reaction pathway finding; computational modeling of chemical reactions	Practice 2 report due
10/10 (Th)	Practice 3: Vibrational frequency analysis and chemical reaction modeling*	First draft of project proposal due (grad students only)
10/15 (Tu)	Implicit solvent models	In-Class Quiz 2
10/17 (Th)	DFT-based methods for electronic excited states	Practice 3 report due
10/22 (Tu)	TD-DFT benchmarks; analysis and visualization tools for ground- and excited-state calculations	
10/24 (Th)	Practice 4: Chemical reactions in solvation environment; excited-state calculations and analysis	Finalized project proposal due (grad students only)
10/29 (Tu)	Electron correlation; configuration interactions (CI) and Møller-Plesset second-order perturbation theory (MP2)	
10/31 (Th)	Coupled cluster (CC) theory and multireference methods in a nutshell; energy decomposition analysis	Practice 4 report due
11/05 (Tu)	Energy decomposition analysis (cont'd)	In-Class Quiz 3
11/07 (Th)	Practice 5: Correlated wavefunction methods; energy decomposition analysis	
11/12 (Tu)	Molecular dynamics (MD) simulations: fundamental theory and practical aspects	All groups should decide which paper to present by this date
11/14 (Th)	MD simulations: fundamental theory and practical aspects (cont'd)	Practice 5 report due
11/19 (Tu)	Preparation and analysis of MD simulations for biomolecular systems	
11/21 (Th)	Practice 6: MD simulations	
11/26 (Tu)	Application of machine learning in computational chemistry; Practice 6 cont'd	
11/28 (Th)	Thanksgiving (no class)	
12/03 (Tu)	Journal club presentations: *Computational chemistry empowered through diversity* (section 1)	Practice 6 report due; In-Class Quiz 4
12/05 (Th)	Journal club presentations: *Computational chemistry empowered through diversity* (section 2)	
12/10 (Tu)	Journal club presentations: *Computational chemistry empowered through diversity* (section 3); class discussion and concluding remarks	
12/12 (Th)	No final exam	
12/17 (Tu)	Final project report due (graduate students only)	

***** The instructor will be giving a seminar at the University of Pittsburgh on Oct. 10. Arrangement for Practice 3 scheduled on that day will be announced later.

Note: This schedule is only *tentative* (primarily to show you what will be covered in this course). Important adjustments to the schedule will be posted on Canvas under "Announcements".

Course Materials:

- Textbook: *Introduction to Computational Chemistry*, 3rd edition, Frank Jensen (Wiley). The textbook is s*trongly recommended but not mandatory*. Its electronic version can be purchased from the SDSU Bookstore (link) and is available in SDSU library (link).
- Course notes/slides and additional learning materials including relevant research papers, reviews, book chapters, tutorial videos, and webinars will be posted on Canvas. If the technical condition allows, the instructor will record the lectures on Zoom and the recordings will also be shared on Canvas.
- You will need to install IQmol, the graphical user interface of Q-Chem, on your personal computer, which will be needed for the practice sessions and the class project. The instructor assumes that all students can bring their own laptops to the practice sessions. If you don't have a laptop or can't get IQmol working on it, please ask the instructor for accommodations or technical support.
- You will also need a software tool to visualize your MD simulations. We will use VMD for this purpose, which also need to be installed on your personal computer.
- You will get temporary access to on-campus or external computer servers/clusters for calculations required for the practice sessions and class projects. Detailed instructions will be provided on Canvas later.

Grading Schemes:

For a 500-level course open to both graduate and undergraduate students, the instructor is required to impose higher requirements on graduate students. In this course, the computational project is required for the graduate students *only*. Undergraduate students will gain experience with the computational tools through the practice sessions but are not required to complete an additional project.

Grading scheme for **graduate students**:

- Quizzes 10%
- Practice sessions 30%
- Journal club presentation 25%
- Computational project 35%

Grading scheme for **undergraduate students**:

- Quizzes 20%
- Practice sessions 40%
- Journal club presentation 40%

Assessments:

- Quizzes: There will be **4 in-class quizzes** (tentative dates have been set on the schedule) focusing on materials covered in the previous weeks. Questions will be short answer and/or multiple choices, and will emphasize on conceptual understanding of the material

rather than numerical calculation. The length of each quiz will be 10-15 minutes. One lowest score will be dropped when calculating the final grade.

- Practice sessions: This course contains **6 hands-on practice sessions (computational chemistry labs)** in which the students will practice using software to perform electronic structure calculations and MD simulations. The students will work *independently* to complete the exercises following the instructions on the provided handout, filling out the worksheets, and answer the follow-up questions. The handout will need to be submitted *as a lab report*. Each practice will be graded on a **10-point scale**: 2 points for attendance and 8 points for the completeness and correctness of the worksheets and answers to questions. Each student is allowed to have one "grace" absence, in which case the instructor must be notified by email before the lab session, and the student is still required to complete the exercises and submit the report before the lab report is due.
- Journal club presentation: Students will work in **groups of 2** (with a group of one single student if the total number is not even) to read one computational chemistry paper selected from a pool of papers authored by a diverse set of theoretical and computational chemists. The selection of papers must be finalized before **Thursday, Nov. 12**. Each group will then give a **12-min presentation** (plus 2-3 minutes for Q&As) in the "*Computational chemistry empowered through diversity*" journal club, which will take place in the last 3 lecture meetings. The two students in one group must both participate in the presentation and each should speak for ~6 minutes. In cases where only one student from a group presents, the presentation will still be fully considered and may be shortened to 8-9 minutes, while the student who does not present will receive no credit. A pool of papers will be provided by the instructor. Each team's presentation will be graded by both the peer audiences and the instructor (10 points from each). The same grade will be assigned to both group members unless for unusual circumstances. The PDF version of the presentation slides will need to be submitted on Canvas after the presentation is given.
- Computational project (graduate student only): A major assessment in this course for graduate students is the class project. Every graduate student is required to complete a brief computational chemistry study, in which they will get a chance to leverage what they have learned from the lectures and practice sessions to investigate topics they are interested in and to potentially add a computational component to their own research. Computational resources will be provided for students to complete these projects (details will be provided later). The total score of this project is 35 points, which will be split into the following two parts:
    - Proposal (5+10=15 points): Every graduate student must submit a proposal (2 pages maximum) for the project before **Thursday, Oct. 10**. The proposal should contain: (1) a descriptive title; (2) background and significance; (3) the scope of chemical system(s) to be investigated; (4) the objectives and approaches; (5) an estimated timeline. The instructor will return the proposal with comments, and the students will be required to revise their draft accordingly and submit the finalized version by **Thursday, Oct. 24** (2 weeks after the first due date).
    - Final project report (20 points): Every graduate student is required to submit a final report (5 pages maximum excluding references) for their class project. It should contain the following components: (1) introduction; (2) computational

details; (3) presentation and discussion of the computational results; (4) conclusions and outlooking; (5) references. The overall scientific writing will also be evaluated. The project report is due on **Tuesday, Dec. 17**.

Note: Detailed grading rubrics for the journal presentations and computational projects will be provided on Canvas when the assignments are created.

Student teams:

The student teams for the journal club presentations will be formed as follows: the instructor will create a Google spreadsheet that contains a list of computational chemistry papers, which is equal to half of the number of students (if the total number of students is not even, one of the teams will have only one students). The students will then select the papers they would like to present and write down their names in the columns next to the paper titles. Note that each paper can at most be presented by 2 students and the slots will be filled on a first-come-first-serve basis.

Tentative grading scale:

Letter	% Cutoff	Letter	%Cutoff
A	90	C	60
A-	85	C-	55
B+	80	D+	50
B	75	D	45
B-	70	D-	40
C+	65	F	<40

Note: The grading scale above is only a rough example. Your final grade will be influenced by the overall class grade distribution to reflect your rank in comparison with your peers.

Late Policy:

If your submission is late by

- 0-2 hours: grace period; no deduction
- 2-24 hours: 20% deduction
- Every 24 hours past due: deducting 20% of the total *in addition to* the initial 20% deduction

For example, under this rule there will be a 40% deduction if your submission is late by 30 hours, and a 60% deduction if late by 50 hours, and so forth. Please try your best to submit your work in time!

Note: The deduction due to late submission may be waived upon the instructor's approval if (i) the instructor is informed in a written form (e.g., email) **before** the assignment is due and (ii) there is a legit, excusable reason (based on the instructor's judgment) for not being able to turn in the work on time.

Academic honor code:

Students are expected never to represent someone else's work as their own or assist others in doing so. Violations of this rule will be documented and may result in automatic failure and

disciplinary review by the University. Please see the SDSU academic honesty page for further information.
Note: while you are allowed to discuss with your peers to complete the tasks in the practice sessions, you should never duplicate the numerical results from others' work. Those duplications are usually quite easy to find out.

Because of the collaborative nature of the journal presentation task, students should strictly follow the instructions so that they can adhere to the academic honor code while being effective team players.

Essential student information:
For essential information about student academic success, please see the SDSU Student Academic Success Handbook.

- SDSU provides disability-related accommodations via the Student Ability Success Center (sascinfo@sdsu.edu | sdsu.edu/sasc). Please allow 10-14 business days for this process.
- Class rosters are provided to the instructor with the student's legal name. Please let the instructor know if you would prefer an alternate name and/or gender pronoun.

Land acknowledgment:
For millennia, the Kumeyaay people have been a part of this land. This land has nourished, healed, protected and embraced them for many generations in a relationship of balance and harmony. As members of the San Diego State University community, we acknowledge this legacy. We promote this balance and harmony. We find inspiration from this land, the land of the Kumeyaay.

Diversity, equity, and inclusion:
We, at SDSU, value the diverse identities of our students, faculty, and staff, which include but are not limited to the differences in race, gender, ethnicity, sexual orientation, age, socioeconomic status, religion, and disability. We will work together to promote diversity, equity, and inclusion in our learning environment, not only for academic excellence but also for social justice. The instructor is committed to adopt an inclusive teaching approach to help students from diverse backgrounds succeed in this course. Discussions in which different perspectives and opinions are respected and valued are encouraged inside and outside the classroom.