Chem-596: Computational Chemistry: Spring 2023

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Lecture Meetings: Tuesday, Thursday 5:00-6:15pm, GMCS-329
Practice sessions: Same as lecture time; location: GMCS-329 or GMCS-245 (TBA)
Office hours: Tuesday 1-2pm & Thursday 11am-noon, or by appointment
Prerequisite: CHEM-410A (not mandatory but 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 package and start running a quantum chemistry calculation or MD simulation, it requires knowledge and skills to set up calculations that can provide reasonably accurate results within a reasonable amount of time. There are common pitfalls that one should do their best to avoid. Our course will cover both the *fundamental principles* and *practical aspects* of each computational method introduced: besides *lectures*, there will be *practice sessions* (computer labs) in which students will gain hands-on experience on setting up and running calculations and analyzing the results. In addition, students will work in teams to complete a more comprehensive *computational project*, through which they are expected to practice the knowledge and skills they learned in this class.

Student Learning Objectives:

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

- Discover what state-of-the-art computational chemistry can achieve and explore how computations/simulations can benefit their own research

- Understand the basic ideas underlying the modern electronic structure methods covered in this course and the strengths and weaknesses of each method; know how to select an appropriate level of electronic structure theory for a given system and properties to compute and how to incorporate the environment effects in electronic structure calculations
- Set up Q-Chem calculations to predict energies, molecular structures, reactivities, non-covalent interactions, and various types of spectra such as UV-Vis and IR; execute Q-Chem (and other software packages) on a Linux server/cluster; utilize analysis and visualization tools to interpret the results of quantum chemistry calculations
- Grasp the basic principles and practical aspects of molecular dynamics (MD) simulations; set up MD simulations for simple solute-solvent systems and large biomolecules; compute static and dynamical properties from MD trajectories obtained
- Understand and evaluate journal papers reporting a full computational study of a given chemical problem or a series of chemical systems; extract useful information regarding how to select computational methods from benchmark studies of various computational methods
- Recognize and appreciate the essential role of diversity, equity, and inclusion in the progression of the field of computational chemistry

Tentative course calendar:

Date	Content	Note
01/19 (Th)	Course info; introduction to computational chemistry	
01/24 (Tu)	Quantum mechanics recap; variational method	
01/26 (Th)	Born-Oppenheimer Approximation; electronic Hamiltonian; many-electron wavefunctions	
01/31 (Tu)	Hartree-Fock theory and self-consistent field (SCF) calculations	
02/02 (Th)	Hartree-Fock wrap-up; introduction to IQmol	
02/07 (Tu)	Atomic basis sets in quantum chemistry	
02/09 (Th)	Practice 1: Building molecules using IQmol; Hartree-Fock energy calculations; basis set convergence	Rough project ideas due
02/14 (Tu)	Basic principles of density functional theory (DFT)	Practice 1 report due; student teams assigned
02/16 (Th)	“Jacob’s ladder” for density functionals; dispersion corrections in DFT; examples of DFT benchmark studies	
02/21 (Tu)	DFT wrap-up; nuclear forces and geometry optimization	
02/23 (Th)	Practice 2: DFT calculations and geometry optimization	
02/28 (Tu)	Harmonic frequency calculations; transition state search; reaction pathway finding	Practice 2 report due
03/02 (Th)	Solvation models; multiscale modeling techniques in a nutshell	Project proposal (first draft) due

03/07 (Tu)	Practice 3: Modeling chemical reactions using quantum chemistry calculations; prediction of IR spectra	
03/09 (Th)	DFT-based methods for electronic excited states	
03/14 (Tu)	Analysis and visualization tools for ground- and excited-state calculations	Practice 3 report due
03/16 (Th)	Electron correlation; configuration interactions (CI) and Møller-Plesset second-order perturbation theory (MP2)	Revised project proposal due
03/21 (Tu)	Coupled cluster (CC) theory and multireference methods in a nutshell	
03/23 (Th)	Practice 4: Excited-state calculations and analysis	
03/28 (Tu)	Spring Break	
03/30 (Th)	Spring Break	
04/04 (Tu)	Special topic 1: unraveling non-covalent interactions (NCIs) using quantum chemistry calculations	Practice 4 report due
04/06 (Th)	Practice 5: Energy decomposition analysis of NCIs	Each group should decide which paper to present by this date
04/11 (Tu)	Molecular dynamics (MD) simulations: fundamental theory and concepts	
04/13 (Th)	Practical aspects of MD simulations: integrators, thermostats, force field parameters, etc.; commonly used MD packages	Practice 5 report due
04/18 (Tu)	Preparation and analysis of MD simulations for condensed-phase systems	
04/20 (Th)	Practice 6: MD simulation for biomolecules	
04/25 (Tu)	Special topic 2: application of machine learning in computational chemistry	
04/27 (Th)	Journal club presentations: *Computational chemistry empowered through diversity* (section 1)	Project 6 report due
05/02 (Tu)	Journal club presentations: *Computational chemistry empowered through diversity* (section 2)	
05/04 (Th)	Journal club presentations: *Computational chemistry empowered through diversity* (section 3); class discussion and concluding remarks	
05/11 (Th)	No final exam	Class project report due (before mid-night)

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).
- 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 (if you plan to do electronic structure calculations). 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. Unless otherwise noted later in this course, we will use VMD for this purpose.

Grading scheme:

- Practice sessions (30%): This course contains **6 practice sessions (computational chemistry labs)** in which the students will practice using software to perform electronic structure calculations and MD simulations. Each student will work *independently* to complete the exercises following the instructions on the given 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**: 3 points for attendance and 7 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. Overall, these will take up 30% of your final score of this course (5% per practice session).
- Journal club presentation (20%): Students will work in **groups of 2** 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, 04/06**. 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 our last 3 lecture meetings. The two students in one group must both participate in the presentation and each should speak for ~6 minutes. Failure to do so will result in a 50% deduction of the sole presenter's score and a zero for the student who doesn't present (except for special scenarios that are acknowledged by the instructor). The pool of papers will be provided by the instructor, which will contain ~20 papers (above the total number of groups by a significant margin). Your presentation will be graded by both your peer audiences and the instructor (10 points from each). The PDF version of your presentation slides will need to be submitted on Canvas after the presentation is given.

- Computational project (50%): Another major event in this course is the class project. Students will work in **groups of 2** to complete a computational chemistry study in which they will get a chance to leverage what they learned from the lectures and practice sessions to investigate topics they are interested in and to assist in their own research. Computational resources on campus will be provided for students to complete these projects (details will be provided later). The total score of this project is 50 points, which will be split into the following two parts:
    - Proposal (15 pts): The two students in each group must submit a proposal (2 pages maximum) jointly for the project before **Thursday, March 2**. The proposal should contain: (1) a descriptive title; (2) background and significance; (3) the chemical system(s) to investigate and an execution plan; (4) the objectives to be achieved. The instructor will return the proposal with comments, and each group will need to submit their revised (final) proposal before **Thursday, March 16** (2 weeks after the first due date).
    - Final written report (35 pts): Each group is required to submit a final report (5 pages maximum excluding references) for their class project. Both students must be involved in the writing process and the work should be distributed as evenly as possible. One recommended way to split the work:
        - Student 1: Introduction; results and discussion
        - Student 2: Computational method; compilation of figures and tables

      You are encouraged to edit each other's work afterwards to improve the quality of writing and to make sure that references are added properly. The final draft should then include a small section listing each author's contribution (which is usually called "Author Contributions" in journal papers). This is actually pretty similar to how collaborative research papers are written in the real world. The project report is due on **Thursday, May 11** (the last of the final exams).

Further instructions and the detailed grading rubrics for each of these modules will be provided later on Canvas.

Student teams:

The student teams will be formed as follows:

- The instructor will create a Google spreadsheet
- All graduate students in this course are *required* to write down some rough ideas on what they would like to do for the class project; undergraduate students who would like to contribute research ideas are encouraged to do so as well (with a 3-point bonus added to the project grade). The ideas need to be submitted before **Thursday, 02/09**. In the case that we don't have enough ideas, the instructor will provide a few topics for you to choose from.
- Undergraduate students who haven't written down an idea should then pick one that you would like to work on. Each team can only have 2 students so the ideas will be selected on a first-come-first-serve basis.

- For students who haven't put down their names in the spreadsheet by the end of **Tuesday, 02/14**, the instructor will assign them into teams. In the case that the total number of students is not even, one of the teams will have 3 students.

Note: The ideas can be adjusted or even significantly modified after discussions with your teammates; the proposal will be the formal version of research ideas.

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: 5% deduction
- Every 24 hours past due: deducting 10% of the total *in addition to* the initial 5% deduction

For example, under this rule there will be a 15% deduction if your submission is late by 30 hours, and a 25% deduction if late by 50 hours, and so forth.

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.

Because of the collaborative nature of a large portion of the assignments (journal club presentation and computational project) in this course, students should follow the instructions for those assignments 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.