



College of Arts & Sciences
Computational Chemistry - CHEM 4359 Syllabus

Instructor: Dr. Yulun Han
Office: STEM 311J
Office Hours: F 2:00 – 3:00 pm
Email: yulun.han@tamusa.edu

Class Hours: F 8:00-10:45 am
Class Location: STEM 121
Phone: 210-784-2674

Course Description

This entry-level course introduces computational chemistry, blending essential theoretical knowledge with practical skills to address chemical problems using computational tools. The course is tailored for students without a background in quantum mechanics or advanced mathematics, focusing on the application of software to run simulations rather than exploring mathematical details.

Prerequisite: MATH 1314, CHEM 1311, CHEM 1312.

Learning Objectives

By the end of this course, successful students will:

1. Comprehend key concepts in computational chemistry
2. Apply computational techniques
3. Leverage high-performance computing
4. Visualize and communicate molecular insights
5. Develop and complete a research project

Communication: The best way to contact instructors is via email. All correspondence between professors and students must occur via Texas A&M University - San Antonio email accounts. Students are expected to access Blackboard regularly for updates on the course, announcements, and other course materials. All students are strongly encouraged to come to office hours or make appointments at other times to discuss course material and ask questions. Discussions concerning grading/grades will not be addressed through email and will only be discussed during office hours or scheduled appointments.

Attendance Policy: All students are expected to attend lecture and actively engage in class discussion, activities, and online assignments. Attendance will be monitored and can be used to make decisions on cases of borderline grades. If you are absent, you are responsible for the material covered and are expected to get notes, announcements and any other material from another student in the class. Absences will be excused if due to illness (medical excuse), death of a close family member, religious holiday (please inform instructor), official university activity or cancellation of classes, military duties, pregnancy & related conditions and participation in legal proceedings. Excessive absences (more than 3) and tardiness will not be tolerated. Accumulation of more than three unexcused absences will result in the student being dropped from the class or in one letter lecture grade decrease at the discretion of the instructor.

Conduct and Behavior: My goal is to create a safe and engaging learning environment. Class disruptions are unacceptable, asking questions to clarify material during class does not qualify as a disruption and is

encouraged. If you disrupt the class, you will be asked to leave for the day. Technology in the classroom may be a great a resource but it can also hinder the learning process. Therefore, students are not allowed to wear ear buds and headphones and/or use cellphones during class. All cellphones must be on vibrate or turned off for the entirety of the class/lab period. In case of an emergency call, leave the room before answering the call. Texting during class is absolutely prohibited. The use of laptops, tablets or other devices for non-class related activities is not allowed. Electronic Devices during Exams. All electronic devices must be completely stored during exams and quizzes. Academic misconduct and attempts to cheat during the exam will be pursued according to Texas A&M-San Antonio code of conduct policy. You are discouraged from leaving the room during an exam. If you need to use the restroom, ask and leave all electronic devices with the instructor. Aggressive Behavior. The academic environment is meant for discussing ideas in a respectful manner. Tolerance, empathy, respect, and courtesy help us create a safe environment. Abusive and aggressive behavior will result in contacting the University Police Department and immediate removal of the student from the classroom. Visitors. Only students enrolled in the course are allowed in the classroom. No visitors are allowed. **IMPORTANT.** Each student receives this information during the first lecture. It is your responsibility to read this material and be familiar with the course content, procedures, and grading.

Tentative schedule*

Week	Week of	Topic
1	Jan 20	Introduction
2	Jan 27	Applications in Computational Chemistry
3	Feb 3	Mathematics, Linux, Using HPC systems
4	Feb 10	Software Installation and Visualization Tools
5	Feb 17	Molecular Orbital Theory I
6	Feb 24	Molecular Orbital Theory II
7	Mar 3	Basis Sets I
8	Mar 10	Spring break
9	Mar 17	Basis Sets II
10	Mar 24	Geometry Optimization
11	Mar 31	Density functional theory
12	Apr 7	Calculating molecular properties
13	Apr 14	Transition state
14	Apr 21	Molecular Dynamics Simulation
15	Apr 28	Excited State and UV-Vis Spectroscopy
16	May 7-13	Presentation/Project

***Note:** Subject to change (Dates, topics, homework and exam coverage are tentative. The instructor reserves the right to make changes as deemed necessary.) Please check your course announcement on blackboard regularly.

Grading: Your course grade will be determined by three components i.e. final project, report, and presentation, each worth 100 points. These are the only opportunities for you to earn points throughout the semester.

$$\% \text{ of Total Points: } \left(\frac{\text{You total points}}{300} \right) \times 100$$

All grades will be posted to Blackboard. However, course percentages, letter grades, etc. are not to be considered as official and students should use caution when using those to evaluate overall course grades. To calculate your grade, use the equation above. Using that equation, letter grades will be determined as:

Letter Grades:	A:	90.0 - 100%
	B:	80.0 - 89.9%
	C:	70.0 - 79.9%
	D:	60.0 - 69.9%
	F:	0 - 59.9%

Note: I will only discuss your grade in person and only with you. I will not discuss your grade through email, by phone call, etc.

Final project: Develop and complete a computational chemistry research project, demonstrating the application of techniques and tools learned during the course.

Report: You are required to submit a short journal-style report (6 to 10 pages), due two weeks before the final exam day. The report must be written in the ACS journal style format. The report must include the following sections:

- A. Title.
- B. Author and affiliation.
- C. Abstract.
- D. Introduction.
- E. Methods.
- F. Results and Discussion.
- G. Conclusion.
- H. References.
- I. Supporting information.

Peer Review: In addition to submitting your report, you can participate in a peer review process. The instructor (i.e. editor) will assign you one or more final reports from other classmates to review. You will need to provide constructive feedback. Both the instructor's comments and your peer review comments will be returned to the author. This process not only helps your classmates improve but also enhances your critical thinking and understanding. Students who participate in the peer review process can earn up to 50 points of extra credit, depending on the quality of their comments. The more insightful, constructive, and detailed your feedback, the higher the points you can earn.

Reviews and Revisions: Manuscripts are rarely accepted for publication in a journal without requiring some revisions by the authors. Similarly, you will have the opportunity to revise and resubmit your final report for a better grade. To do so, you **MUST** append the original graded report to your revised submission and include a brief "Letter to the Editor" explaining how you addressed the initial comments (from the Editor and peer reviewer, if applicable). However, please note that the opportunity to revise may or may not be granted by "the Editor", depending on the quality of your original report.

Presentation: You are required to deliver a 30-minute presentation on your final project. The presentation should effectively summarize your research, highlight key findings, and discuss their significance. It is an opportunity to demonstrate your understanding of computational chemistry concepts and communicate your work in a professional setting.

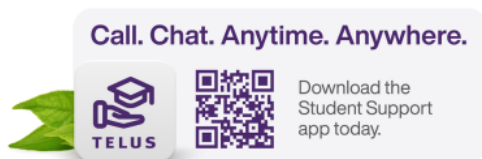
IMPORTANT POLICIES AND RESOURCES

Academic Accommodations for Individuals with Disabilities: Texas A&M University-San Antonio is committed to providing all students with reasonable access to learning opportunities and accommodations in accordance with The Americans with Disabilities Act, as amended, and Section 504 of the Rehabilitation Act. If you experience barriers to your education due to a disability or think you may have a disability, Disability Support Services is located in the Central Academic Building, Suite 210. You can also contact us via phone at (210) 784-1335, visit us <https://www.tamusa.edu/Disability-Support-Services/index.html> or email us at dss@tamusa.edu. Disabilities may include, but are not limited to, attentional, learning, mental health, sensory, physical, or chronic health conditions. All students are encouraged to discuss their disability-related needs with Disability Support Services and their instructors as soon as possible.

Academic Learning Center: The Academic Learning Center provides free course-based tutoring to all currently enrolled students at Texas A&M University-San Antonio. Students wishing to work with a tutor can make appointments through the Brainfuse online tutoring platform. Brainfuse can be accessed in the *Tools* section of Blackboard. You can contact the Academic Learning Center by emailing tutoring@tamusa.edu, calling (210) 784-1307, or visiting the Central Academic Building, room 202.

Counseling/Mental Health Resources: As a college student, there may be times when personal stressors interfere with your academic performance and negatively impact your daily functioning. If you are experiencing emotional difficulties or mental health concerns, support is available to you through the Student Counseling Center (SCC). To schedule an appointment, call 210-784-1331 or visit Madla 120. All mental health services provided by the SCC are free and confidential (as the law allows). The Student Counseling Center provides brief individual and group therapy, crisis intervention, consultation, case management, and prevention services. For more information on SCC services visit tamusa.edu/studentcounseling

Crisis support is available 24/7 by calling the SCC at 210-784-1331 (after-hours select option '2'). Additionally, the TELUS Student Support App provides a variety of mental health resources to including support for in the moment distress, an anonymous peer to peer support network, mental health screenings, podcasts, and articles to improve your mental wellbeing.



Emergency Preparedness: JagE Alert is Texas A&M University-San Antonio's mass notification. In the event of an emergency, such as inclement weather, students, staff and faculty, who are registered, will have the option to receive a text message, email with instructions and updates. To register or update your information visit: <https://tamusa.bbcportal.com/>.

More information about Emergency Operations Plan and the Emergency Action Plan can be found here: <https://www.tamusa.edu/about-us/emergency-management/>.

Download the SafeZone App (<https://safezoneapp.com/>) for emergencies or call (210) 784-1911. Non-Emergency (210) 784-1900.

Financial Aid and Verification of Attendance: According to the following federal regulation, 34 CFR 668.21: U.S. Department of Education (DoE) Title IV regulation, a student can only receive Title IV funds

based on Title IV eligibility criteria which include class attendance. If Title IV funds are disbursed to ineligible students (including students who fail to begin attendance), the institution must return these funds to the U.S. DoE within 30 days of becoming aware that the student will not or has not begun attendance. Any student receiving federal financial aid who does not attend by the census date will have their financial aid terminated and returned to the DoE. Please note that any student who stops attending at any time during the semester, a Care report will be submitted, and you will possibly be dropped from the class. Your financial aid may have to be recalculated and a portion of your federal aid may have to be returned to the DoE.

Writing, Language, and Digital Composing Center: The Writing, Language, and Digital Composing Center supports graduate and undergraduate students in all three colleges as well as faculty and staff. Tutors work with students to develop reading skills, prepare oral presentations, and plan, draft, and revise their written assignments. Our language tutors support students enrolled in Spanish courses and students composing in Spanish for any assignment. Our digital studio tutors support students working on digital projects such as eportfolios, class presentations, or other digital multimedia projects. Students can schedule appointments through JagWire under the Student Services tab. Click on “Writing, Language, and Digital Composing Center” to make your appointment. The Center offers face-to-face, synchronous online, and asynchronous digital appointments. More information about what services we offer, how to make an appointment, and how to access your appointment can be found on our website at <https://www.tamusa.edu/academics/>.

Meeting Basic Needs: Any student who has difficulty affording groceries or accessing sufficient food to eat every day or who lacks a safe and stable place to live, and believes this may affect their performance in the course, is urged to submit a CARE referral (<https://www.tamusa.edu/university-policies/Student-Rights-and-Responsibilities/file-a-report.html>) for support. Furthermore, please notify the professor if you are comfortable in doing so. This will enable them to direct you to available resources.

Military Affairs: Veterans and active-duty military personnel are welcomed and encouraged to visit the Office of Military Affairs for any question involving federal or state VA Education Benefits. Visit the Patriots’ Casa building, room 202, or to contact the Office of Military Affairs with any questions at military.va@tamusa.edu or (210)784-1397.

Religious Observances: Texas A&M University-San Antonio recognizes the diversity of faiths represented among the campus community and protects the rights of students, faculty, and staff to observe religious holidays according to their tradition. Under the policy, students are provided an opportunity to make up any examination, study, or course work requirements that may be missed due to a religious observance provided they notify their instructors before the end of the second week of classes for regular session classes.

The Six-Drop Rule: Students are subject to the requirements of Senate Bill (SB) 1231 passed by the Texas Legislature in 2007. SB 1231 limits students to a maximum of six (6) non-punitive course drops (i.e., courses a student chooses to drop) during their undergraduate careers. A non-punitive drop does not affect the student’s GPA. However, course drops that exceed the maximum allowed by SB 1231 will be treated as “F” grades and will impact the student’s GPA.

Statement of Harassment and Discrimination: Texas A&M University-San Antonio is committed to the fundamental principles of academic freedom, equal opportunity, and human dignity. To fulfill its multiple missions as an institution of higher learning, A&M-San Antonio encourages a climate that values and

nurtures collegiality and the uniqueness of the individual within our state, nation, and world. All decisions and actions involving students and employees should be based on applicable law and individual merit. Texas A&M University-San Antonio, in accordance with applicable federal and state law, prohibits discrimination, including harassment, on the basis of race, color, sex, religion, national origin, age, disability, genetic information, veteran status, sexual orientation, gender identity, gender expression, or pregnancy/parenting status. Individuals who believe they have experienced harassment or discrimination prohibited by this statement are encouraged to contact the appropriate offices within their respective units.

Texas A&M University-San Antonio faculty are committed to providing a safe learning environment for all students and for the university as a whole. If you have experienced any form of sex- or gender-based discrimination or harassment, including sexual assault, sexual harassment, domestic or dating violence, or stalking, know that help and support are available. A&M-San Antonio's Title IX Coordinator can support those impacted by such conduct in navigating campus life, accessing health and counseling services, providing academic and housing accommodations, and more. The university strongly encourages all students to report any such incidents to the Title IX Coordinator. Please be aware that all A&M-San Antonio employees (other than those designated as confidential resources such as counselors and trained victim advocates) are required to report information about such discrimination and harassment to the university. This means that if you tell a faculty member about a situation of sexual harassment, sexual violence, or other related misconduct, the faculty member must share that information with the university's Title IX Coordinator (titleix@tamusa.edu, 210-784-2061, CAB 439K). If you wish to speak to a confidential employee who does not have this reporting requirement, you can contact the Student Counseling Center at (210) 784-1331 or visit them in Madla 120.

Pregnant/Parenting Students: Texas A&M-San Antonio does not require a pregnant or parenting student, solely because of that status or issues related to that status, to (1) take a leave of absence or withdraw from their degree or certificate program; (2) limit the student's studies; (3) participate in an alternative program; (4) change the student's major, degree, or certificate program; or (5) refrain from joining or cease participating in any course, activity, or program at the University. The university will provide such reasonable accommodations to pregnant students as would be provided to a student with a temporary medical condition that are related to the health and safety of the student and the student's unborn child. These could include maintaining a safe distance from substances, areas, and activities known to be hazardous to pregnant individuals and their unborn child; excused absences because of illness or medical appointments; modified due dates for assignments; rescheduled tests/exams; taking a leave of absence; and being provided access to instructional materials and video recordings of lectures for excused absences, if these would be provided to any other student with an excused absence. Pregnant/parenting students are encouraged to contact the Title IX Coordinator with any questions or concerns related to their status (titleix@tamusa.edu; 210-784-2061; CAB 439K). Texas A&M-San Antonio has also designated the Title IX Coordinator as the liaison officer for current or incoming students who are the parent or guardian of a child younger than 18 years of age. The Title IX Coordinator can provide students with information regarding support services and other resources.

Students' Rights and Responsibilities: The following statement of students' rights and responsibilities is intended to reflect the philosophical base upon which University Student Rules are built. This philosophy acknowledges the existence of both rights and responsibilities, which is inherent to an individual not only as a student at Texas A&M University-San Antonio but also as a citizen of this country.

Students' Rights

1. A student shall have the right to participate in a free exchange of ideas, and there shall be no University rule or administrative rule that in any way abridges the rights of freedom of speech, expression, petition and peaceful assembly as set forth in the U.S. Constitution.
2. Each student shall have the right to participate in all areas and activities of the University, free from any form of discrimination, including harassment, on the basis of race, color, national or ethnic origin, religion, sex, disability, age, sexual orientation, gender identity, gender expression, and pregnancy/parenting or veteran status in accordance with applicable federal and state laws.
3. A student has the right to personal privacy except as otherwise provided by law, and this will be observed by students and University authorities alike.
4. Each student subject to disciplinary action arising from violations of university student rules shall be assured a fundamentally fair process.

Students' Responsibilities

1. A student has the responsibility to respect the rights and property of others, including other students, the faculty, and administration.
2. A student has the responsibility to be fully acquainted with the published University Student Rules found in the Student Handbook, [Student Code of Conduct](#), on our website, and University Catalog, and to comply with them, as well as with federal, state, and local laws.
3. A student has the responsibility to recognize that student actions reflect upon the individuals involved and upon the entire University community.
4. A student has the responsibility to recognize the University's obligation to provide a safe environment for learning.
5. A student has the responsibility to check their university email for any updates or official university notifications.

We expect that students will behave in a manner that is dignified, respectful, and courteous to all people, regardless of sex, ethnic/racial origin, religious background, sexual orientation, or disability. Conduct that infringes on the rights of another individual will not be tolerated.

Students are expected to exhibit a high level of honesty and integrity in their pursuit of higher education. Students engaging in an act that violates the standards of academic integrity will find themselves facing academic and/or disciplinary sanctions. Academic misconduct is any act, or attempt, which gives an unfair advantage to the student. Additionally, any behavior specifically prohibited by a faculty member in the course syllabus or class discussion may be considered as academic misconduct. For more information on academic misconduct policies and procedures please review the Student Code of Conduct (<https://www.tamusa.edu/university-policies/student-rights-and-responsibilities/documents/Student-Handbook-2022-23.pdf>) or visit the resources available in the OSRR website (<https://www.tamusa.edu/university-policies/student-rights-and-responsibilities/academic-integrity.html>).

Use of Generative AI Permitted Under Some Circumstances or With Explicit Permission

There are situations and contexts within this course where you may be asked to use artificial intelligence (AI) tools to explore how they can be used. Outside of those circumstances, you should not use AI tools to generate content (text, video, audio, images) that will end up in any student work (assignments, activities, discussion responses, etc.) that is part of your evaluation in this course. Any student work submitted using AI tools should clearly indicate with attribution what work is the student's work and what part is generated by the AI. In such cases, no more than 25% of the student work should be generated by AI. If any part of this is confusing or uncertain, students should reach out to their instructor for clarification before submitting work for grading. Use of AI-generated content without the instructor's

permission and/or proper attribution in this course qualifies as academic dishonesty and violates Texas A&M-San Antonio's standards of academic integrity.

NOTE: Guidance for how to cite AI-generators, like ChatGPT, can be found here

<https://apastyle.apa.org/blog/how-to-cite-chatgpt>

Important Dates:

Jan 21	First day of class
April 21	Last day to drop with an automatic "W"
April 28	Last day to drop a course or withdraw from the University
May 5	Last day of classes
May 7-13	Final exams

The complete academic calendar is available online: <https://www.tamusa.edu/academics/academic-calendar/index.html>