CHEM 418 — CHEM 518

COMPUTATIONAL CHEMISTRY
for Experimentalists and Non-Experts

Spring 2023

Biological Sciences West (BSW) — Room 251

Days and Time

Tu-Th 11:00 AM – 12:15 PM

Instructor Information

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Course Description

Quantum chemistry (QC) codes are increasingly exploited to calculate the geometric and electronic structures of molecules and materials and thereby gain access to, for instance, their optical, electrical, vibrational, or magnetic properties. They provide tools to obtain useful theoretical interpretation of experimental data and/or to guide the development of novel promising molecules or materials.

Codes such as “Gaussian”, “Schrödinger”, “Q-Chem”, or “Spartan”, are now widely available. Especially in the case of commercial codes, they are packaged in such a way as to be easily

accessible for a wide community of scientists and engineers, including experimentalists. The major issue then is that they can be used as push-button black boxes by those not familiar with the basic principles of quantum-chemical methodologies and their limitations. As a consequence, the results of QC calculations can turn out to be dramatically misinterpreted when the users are applying methodologies that are not appropriate.

This course is meant: i) to have students become familiar with the terminology of computers, software, molecular modeling, and chemical computations; ii) to inform students of research topics of high current interest; iii) to give students the working principle of computational chemistry codes; iv) to provide students (whose research is mainly experimental in nature) with the basic understanding and know-how of QC techniques; v) to allow students to gauge the quality and relevance of QC computational work appearing in the literature; and vi) to allow students to carry out with confidence simple calculations relevant to their research work.

Course Format

The course will have the following structure:

• The first section will consist of an overview of the main quantum-chemical techniques. The emphasis will be on the concepts (and not the detailed mathematics) behind solving Schrödinger's equation.

The goal is not to train experts but to help the students identify the proper methodologies and avoid pitfalls, by considering a number of topics of current interest.

The next sections will each consist of three modules:
Module 1: General introduction to the specific field of investigation.
Module 2: Introduction to the technical aspects of the QC methodologies relevant to the field of investigation, description of the limitations of these methodologies and of aspects to be avoided.
Module 3: Hands-on illustrative calculations carried out by the students.

The following topics of investigation will be covered (others could also be considered depending on the students' background):
• Introduction to conjugation in organic molecules with application to electrically conducting polymers and electrochromic materials.
• Molecular materials for light emission (light-emitting diodes for displays and solid-state lighting).
• Organic and hybrid organic-inorganic materials for solar-cell applications.
• Introduction to systems with two-dimensional and three-dimensional periodicities: Covalent Organic Frameworks (COFs) and silicon.

A section will also be devoted to an introduction to the basic concepts of molecular dynamics simulations.

Course Prerequisites

Undergraduate Students: (CHEM 105B, CHEM 142, CHEM 152 or CHEM 162) and (MATH 223 or MATH 254 or CHEM 380) and (PHYS 102/181 or PHYS 141 or PHYS 140 or PHYS 161H) and (CHEM 241A or 242A or 246A).
Graduate Students: B.S. or equivalent degree in Chemistry, Biochemistry, Physics, Chemical Engineering, Materials Science and Engineering or Consent of the instructor.

Learning Outcomes

CHEM 418
By the end of this course, the student will be able to:
• Become familiar with the terminology of computers, software, molecular modeling, and chemical computations.
• Become comfortable in working with electronic media, including communications, databases, bulletin boards, files, programs, etc.
• Survey the fundamental postulates, strengths, limitations, and applications of basic molecular modeling and computational methods.
• Gain knowledge of research topics of high current interest, based on organic molecules and materials.

CHEM 518
In addition to the Learning Outcomes for CHEM 418 shown above, the CHEM 518 student will be able to:
• Evaluate hardware and software for molecular modeling.
• Become skilled with selected tools for computational chemistry and learn their pitfalls.
• Survey the fundamental postulates, strengths, limitations, and applications of basic molecular modeling and computational methods.
• Become familiar with original research using these tools.

Workload Expectations

The lectures and introductions to technical aspects will correspond to 50% of the load and the hands-on applications, to 50%. All modules (see below) will be given during normal class hours.

Required Texts and Materials

There are no specific prerequisites, except for general familiarity with computers. Reading materials (based on recently published manuscripts or book chapters or software manuals) will be freely available.

The students need to have access to a portable computer with a reasonable amount of memory, hard drive space, and fast internet connection.

Assessments

General assignments will take the form of reading recommended papers.
Homework will correspond to submission of quantum-chemical calculations on designated computers and of short reports analyzing the results of the calculations.
There will be two mid-term exams (during normal class hours). The final exam will be cumulative. In each instance, study guides will be provided.

Grading:

First mid-term:	50 points
Second mid-term (cumulative):	75 points
Final (cumulative):	125 points
Homework:	250 points
	Total: 500 points

First mid-term:	Tu. 02/28, during regular class time
Second mid-term:	Tu. 04/04, during regular class time
Final Exam:	Tu. 05/09, 10:30 AM - 12:30 PM

Note: Since CHEM 518 is a graduate course, exams will have at least one additional question compared to exams for CHEM 418.

Grading Scale and Policies

A: 80% of the total points and above
B: between 65 and 79%
C: between 50 and 64%
D: between 40 and 49%
F: below 40%

Make-up exams will only be scheduled with a doctor's note or in consultation with the Dean of Students. Excused absences must be approved 1 week before the exam.

Schedule of Topics and Activities (subject to change)

Section 1: Basic concepts of quantum chemistry – 6 classes
• Module 1:
From the time-independent Schrödinger equation to the ab initio Hartree-Fock equations. Very brief introduction to semi-empirical techniques. Introduction to correlated wave-function methods. Basic principles of Density Functional Theory and Jacob's Ladder.
• Module 2:
Introduction to Linux.
• Module 3:
Hands-on submission of a QC job: Building of the input file and analysis of the output file(s).

Section 2: Conjugation in organic π-conjugated molecules with application to electrically conducting polymers and electrochromic materials – 5 classes

• Module 1:

Introduction to π-conjugated molecules and conducting polymers.

• Module 2:

Introduction to methods of geometry optimizations for neutral, positively charged, and negatively charged molecules; simulation of optical absorption spectra.

• Module 3:

Ground-state geometry optimizations for series of analogous neutral molecules (polyenes, oligothiophenes, oligophenylenes, oligophenylene vinylenes) of increasing length in order to illustrate the impact of conjugation on ionization potential and electron affinity.

Geometry optimizations of the positively charged oligomers.

Comparison of the optical absorption spectra between neutral and charged in order to understand electrochromism.

Section 3: Molecular materials for organic light-emitting diodes (OLEDs) with applications to displays and solid-state lighting – 5 classes

• Module 1:

Introduction to π-conjugated molecular emitters for OLEDs.

• Module 2:

Introduction to methods of geometry optimizations in the excited state for singlets and for triplets; natural transition orbitals; simulation of optical emission spectra.

Illustration of the issue of B3LYP with charge-transfer excited states.

Illustration of the failure of simple DFT to describe a system such as DABNA.

• Module 3:

Hands-on application to fluorescent emitters and TADF emitters.

Section 4: Molecular and polymeric materials for organic solar cells – 5 classes

• Module 1:

Introduction to π-conjugated molecular and polymeric materials for photovoltaic devices.

• Module 2:

Introduction to intermolecular charge-transfer states.

Visualization via NTOs.

Evaluation of binding energies.

• Module 3:

Hands-on application to donor-acceptor complexes.

Section 5: Introduction to calculations on crystalline materials – 5 classes

• Module 1:

Introduction to systems with translation symmetry: From conjugated polymer chains to two-dimensional (2D) covalent organic frameworks (COFs) and silicon.

• Module 2:

Introduction to codes allowing calculations on systems with one, two, or three axes of periodicity.

Introduction to reciprocal space description of the electronic structure.

• Module 3:
Hands-on application to donor-acceptor complexes.

Section 6: Brief introduction to the basic principles of molecular dynamics simulations – 2 classes
This section will be inserted earlier in the term, likely after completion of Section 3 (on 03/21 and 03/23).

Class	**Topic**
01/12	General Introduction — Section 1 - Module 1
01/17	Section 1 - Module 1
01/19	Section 1 - Module 1
01/24	Section 1 - Module 1
01/26	Section 1 - Module 2
01/31	Section 1 - Module 3
02/02	Section 2 - Module 1
02/07	Section 2 - Module 1
02/09	Section 2 - Module 2
02/14	Section 2 - Module 3
02/16	Section 2 - Module 3
02/21	Section 3 - Module 1
02/23	Section 3 - Module 1
02/28	**Mid-term I**
03/02	Section 3 - Module 2
03/14	Section 3 - Module 3
03/16	Section 3 - Module 3
03/21	Section 6 - Module 1
03/23	Section 6 - Module 1
03/28	Section 4 - Module 1
03/30	Section 4 - Module 1

04/04	**Mid-term II**
04/06	Section 4 - Module 2
04/11	Section 4 - Module 3
04/13	Section 4 - Module 3
04/18	Section 5 - Module 1
04/20	Section 5 - Module 1
04/25	Section 5 - Module 2
04/27	Section 5 - Module 3
05/02	Section 5 - Module 3

Class Participation and Absence Policies

Participating in the course and attending lectures and other course events are vital to the learning process. As such, **attendance is expected at all lectures**.
If you anticipate being absent or are unexpectedly absent, please contact Dr. Bredas as soon as possible.

Absences for any sincerely held religious belief, observance, or practice will be accommodated where reasonable.
See: policy.arizona.edu/human-resources/religious-accommodation-policy

Absences pre-approved by the UA Dean of Students (or Dean's designee) will be honored.
See: https://deanofstudents.arizona.edu/absences

To request a disability-related accommodation to this attendance policy, please contact the Disability Resource Center at (520) 621-3268 or drc-info@email.arizona.edu. If you are experiencing unexpected barriers to your success in your courses, the Dean of Students Office is a central support resource for all students and may be helpful. The Dean of Students Office is located in the Robert L. Nugent Building, room 100, or call 520-621-7057.

The UA's policy concerning Class Attendance, Participation, and Administrative Drops is available at: http://catalog.arizona.edu/policy/class-attendance-participation-and-administrative-drop.

Course Communications

General announcements will be made on the course D2L site, and/or via email, and/or at the beginning of each class.

Policy for Students Who Register Late

Students who register late will be required to turn in assignments starting from the time they join the class.

Classroom Behavior Policies

To foster a positive learning environment, students and instructors have a shared responsibility. We want a safe, welcoming, and inclusive environment where all of us feel comfortable with each other and where we can challenge ourselves to succeed. To that end, our focus is on the tasks at hand and not on extraneous activities (e.g., texting, chatting, reading a newspaper, making phone calls, web surfing, etc.).

Confidentiality of Student Records

See: http://www.registrar.arizona.edu/personal-information/family-educational-rights-and-privacy-act-1974-ferpa?topic=ferpa

Incomplete (I) or Withdrawal (W)

Requests for incomplete (I) or withdrawal (W) must be made in accordance with University policies, which are available at:
http://catalog.arizona.edu/policy/grades-and-grading-system#incomplete
and http://catalog.arizona.edu/policy/grades-and-grading-system#Withdrawal.

Dispute of Grade Policy

The acceptable time period for disputing a grade on a homework or exam is two days after the homework or exam has been returned to the student.

Accessibility and Accommodations

At Arizona, we strive to make learning experiences as accessible as possible. If you anticipate or experience barriers based on disability or pregnancy, please contact the Disability Resource Center (520-621-3268, https://drc.arizona.edu/) to establish reasonable accommodations.

Nondiscrimination and Anti-Harassment Policy

At Arizona, we are committed to creating and maintaining an environment free of discrimination. In support of this commitment, the University prohibits discrimination, including

harassment and retaliation, based on a protected classification, including race, color, religion, sex, national origin, age, disability, veteran status, sexual orientation, gender identity, or genetic information. For more information, including how to report a concern, please see: http://policy.arizona.edu/human-resources/nondiscrimination-and-anti-harassment-policy

Code of Academic Integrity

At Arizona, integrity and ethical behavior are expected of every student in all academic work. This Academic Integrity principle stands for honesty in all class work, and ethical conduct in all labs and clinical assignments. This principle is furthered by the Student Code of Conduct and disciplinary procedures established by ABOR Policies 5-308 through 5-404 (see chapter 5), all provisions of which apply to all our students.
See https://deanofstudents.arizona.edu/policies/code-academic-integrity

Note:
Selling class notes and/or other course materials to other students or to a third party for resale is not permitted without the instructor's express written consent. Violations to this and other course rules are subject to the Code of Academic Integrity and may result in course sanctions. Additionally, students who use D2L or UA e-mail to sell or buy these copyrighted materials are subject to Code of Conduct Violations for misuse of student e-mail addresses. This conduct may also constitute copyright infringement.

Threatening Behavior Policy

At Arizona, we seek to promote a safe environment where students and employees may participate in the educational process without compromising their health, safety, or welfare. The Arizona Board of Regents (ABOR) Student Code of Conduct, ABOR Policy 5-308, prohibits threats of physical harm to any member of the University community, including to one's self. Threatening behavior can harm and disrupt the University, its community, and its families.

"Threatening behavior" means any statement, communication, conduct, or gesture, including those in written form, directed toward any member of the University community that causes a reasonable apprehension of physical harm to a person or property. A student can be guilty of threatening behavior even if the person who is the object of the threat does not observe or receive it, so long as a reasonable person would interpret the maker's statement, communication, conduct, or gesture as a serious expression of intent to physically harm.
See: https://policy.arizona.edu/education-and-student-affairs/threatening-behavior-students

Additional Resources for Students

Campus Health
http://www.health.arizona.edu/
Campus Health provides quality medical and mental health care services through virtual and in-

person care.
Phone: 520-621-9202

Counseling and Psych Services (CAPS)
https://health.arizona.edu/counseling-psych-services
CAPS provides mental health care, including short-term counseling services.
Phone: 520-621-3334

The Dean of Students Office's Student Assistance Program
http://deanofstudents.arizona.edu/student-assistance/students/student-assistance
Student Assistance helps students manage crises, life traumas, and other barriers that impede success. The staff addresses the needs of students who experience issues related to social adjustment, academic challenges, psychological health, physical health, victimization, and relationship issues, through a variety of interventions, referrals, and follow up services.
Email: DOS-deanofstudents@email.arizona.edu
Phone: 520-621-7057

Survivor Advocacy Program
https://survivoradvocacy.arizona.edu/
The Survivor Advocacy Program provides confidential support and advocacy services to student survivors of sexual and gender-based violence. The Program can also advise students about relevant non-UA resources available within the local community for support.
Email: survivoradvocacy@email.arizona.edu
Phone: 520-621-5767

Campus Pantry
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 contact the Dean of Students for support. In addition, the University of Arizona Campus Pantry is open for students to receive supplemental groceries at no cost.
Please see their website at: campuspantry.arizona.edu for open times.

Preferred Gender Pronoun

This course affirms people of all gender expressions and gender identities. If you prefer to be called a different name than what is on the class roster, please let me know. Feel free to correct instructors on your preferred gender pronoun. If you have any questions or concerns, please do not hesitate to contact Dr. Bredas directly in class or via email.

If you wish to change your preferred name or pronoun in the UAccess system, please use the following guidelines:

Preferred name: University of Arizona students may choose to identify themselves within the University community using a preferred first name that differs from their official/legal name. A student's preferred name will appear instead of the person's official/legal first name in select

University-related systems and documents, provided that the name is not being used for the purpose of misrepresentation. Students are able to update their preferred names in UAccess.

Pronouns: Students may designate pronouns they use to identify themselves. Instructors and staff are encouraged to use pronouns for people that they use for themselves as a sign of respect and inclusion. Students are able to update and edit their pronouns in UAccess.

More information on updating your preferred name and pronouns is available on the Office of the Registrar site at https://www.registrar.arizona.edu/.

Safety on Campus and in the Classroom

Familiarize yourself with the video available at:
https://ua-saem-aiss.narrasys.com/#/story/university-of-arizona-cert/active-shooter

University Policies

All university policies related to this syllabus are available at:
https://academicaffairs.arizona.edu/syllabus-policies.

Subject To Change Notice

Information contained in this course syllabus, other than the grade and absence policies, may be subject to change with reasonable advance notice, as deemed appropriate by the instructor.

https://registrar.arizona.edu/faculty-staff-resources/room-class-scheduling/schedule-classes/final-exams