CH367 Materials Chemistry: FRI Computational Materials
Spring 2019 (Unique Number: 50294)

**Time and Place:**  
TTh 2:00-3:30; Welch 2.128 and/or Welch 4.132B (location is subject to change)

**Instructor/Research Educator:**  
Dr. Juliana Duncan  
jrduncan@utexas.edu  
Welch 3.426  
Office hours: by appointment

**Course Overview:**  
The purpose of this course is to prepare students for research in computational science and engineering with applications in materials & chemistry research. In this course students will:

1. Learn the foundations of describing solid-state materials;
2. Learn how to computationally express potential energy landscapes of materials and other chemical systems;
3. Learn about the computational tools which exists to model properties of materials and chemical systems; and
4. Gain the skills to develop and implement new computational methods, and apply existing methods to model materials & chemical systems of interest.

These skills will be used to find new catalytic materials for alternative energy technologies, and improve methodologies for predicting material & chemical system properties.

**Course Requirements:**  
Below are some important requirements for this course:

1. **Bring your charged laptops to class.** You will be doing course labs and research on your laptop. A significant portion of class time will be spent on labs. Note that you will not be guaranteed an electrical outlet during class to charge your laptop.
2. Attending class is required. You are allowed to miss three classes per semester. You will not receive points for any additional class missed unless the absence is excused. If at all possible please speak with me about any excused absences before you miss class.

**Lab hours:**  
There will be computational chemistry lab hours available to students where you can work on your assignments with your classmates. Mentors, TAs, or I will also be available to help you with the assignments. The time and place are TBD and will be posted on the stream webpage.

**Course Outline and Computational Chemistry Labs:**  
A series of labs will play an important role in teaching you the course content outlined below. Labs will involve python programming exercises, utilization of DFT software, and customization of individual research webpages. Each student will be responsible for posting all results from labs on their individual webpage. All labs for the course and additional information can be found at the stream’s webpage: [http://fri.cnm.utexas.edu/fri/](http://fri.cnm.utexas.edu/fri/). The due dates for each lab will also be posted on the stream webpage.
Topics covered:

1. Computer Science foundations:
   a. Introduction to Linux, HTML and Python Programming

2. Introduction to generating potential energy landscapes of materials & chemical systems
   a. Electronic Structure Calculations
      i. Introduction to Quantum Mechanics and solving Schrödinger’s equation
      ii. Introduction to Density Functional Theory (DFT)
   b. Empirical potentials
      i. Bonding in solids and intermolecular forces

3. Introductions to Materials & Catalytic Chemical Systems
   a. Nanoparticles
   b. Introduction to crystal structures
      i. Describing crystal structures: unit cells, lattice constants, etc.
      ii. Crystal planes: Miller indices
      iii. Common structures of solids: BCC, FCC, HCP, etc.
      iv. Application → compare structural stability of materials with DFT
   c. Introduction to catalytic materials discovery
      i. Kinetics → rate laws, activation energy, and Arrhenius rates
      ii. Sabatier’s Principle and Volcano Plots
      iii. Application → Calculating binding energies with DFT
         1. Introduction to local optimization

4. Introduction to Statistical Mechanics:
   a. Introduction to Ensembles
   b. Introduction to molecular dynamics (MD) simulations of chemical systems
   c. Introduction to Monte Carlo (MC) simulations of chemical systems
   d. Applications of MD and MC simulations in chemistry:
      i. phase transformations of solids
      ii. benchmark algorithms that predict structure of nanoparticles

Projects:
An independent project will be assigned in the last four weeks of the semester. Students will be required to write a research paper on the results achieved during the course. Students will also give a short presentation on their results. Research projects will be introduced during the semester.

Research Paper:
A research paper will be written at the conclusion of the semester. This paper will include a cover page and at least 6 pages of typed text that is double-spaced with a 1” margin excluding tables and figures, and a bibliography. The report will be in ACS format. Check out this website for useful information on the ACS format (http://pubs.acs.org/isbn/9780841239999). Students will be given a rubric explaining how the paper will be graded. Students will also be required to participate in peer-review exercises. This paper is due on the last day of class (5/9/19) at 2:00pm. Late papers will not be accepted.

Course Grading:
Participation: 10%
Labs: 50%
Projects: 10% oral presentations; 30% written report
Suggested Resources:
Various suggested resources will be given throughout this course and will be posted on the course webpage. All suggested readings will be available for free through UT library or other resources.

Course Webpage:
All important course updates and information can be found on the course webpage:
http://fri.cnm.utexas.edu/fri/

Independent Inquiry:
This course carries the Independent Inquiry flag. Independent Inquiry courses are designed to engage you in the process of inquiry over the course of a semester, providing you with the opportunity for independent investigation of a question, problem, or project related to your major. You should therefore expect a substantial portion of your grade to come from the independent investigation and presentation of your own work.

Writing:
This course carries the Writing Flag. Writing Flag courses are designed to give students experience with writing in an academic discipline. In this class, you can expect to write regularly during the semester, complete substantial writing projects, and receive feedback from your instructor to help you improve your writing. You will also have the opportunity to revise one or more assignments, and you may be asked to read and discuss your peers’ work. You should therefore expect a substantial portion of your grade to come from your written work. Writing Flag classes meet the Core Communications objectives of Critical Thinking, Communication, Teamwork, and Personal Responsibility, established by the Texas Higher Education Coordinating Board.

Academic Integrity:
Cheating is giving or accepting unauthorized aid on assignments. You will be encouraged to work together on assignments, but you should never copy another student’s work or take credit for research results another student produced. Rather, you should have other students help you debug the script you have produced, or discuss a plan for a programming assignment and then create the script separately. An example of cheating would be copying another students code and changing the variable names. Another example would be presenting another students research results as if it was your own without permission from that student and acknowledging the other student’s contribution. Students caught cheating will be given one warning and a significant penalty on the corresponding assignment. The second time, students will get a zero on their assignment.

Classroom Expectations:

Classroom Behavior:
Reading and sending emails (not related to the course), completing work for other courses in class, playing video games, streaming videos, and other activities not related to in class activities is not appropriate. Students engaging in these sorts of activities will be removed from the classroom and will not receive points for attendance that day.

Professionalism:
Students are expected to behave in a professional manner during class. Any comments of a derogatory nature towards other students, mentors, TA, or the instructor will not be tolerated. Students engaging in these sorts of activities will be removed from the classroom. If inappropriate
behaviors occur more than once or are deemed abusive, the incident will be reported to the Student Judicial Services (http://deanofstudents.utexas.edu/sjs/) and will go on the student's permit record.

Disclaimer: The standards and requirements set forth in this syllabus may be modified at any time by the course instructor. Notice of such changes will be by announcement in class or by written or email notice.

Additional University Policies and Resources

Religious Holy Days:

By UT Austin policy, you must notify your instructor of your pending absence at least fourteen days prior to the date of observance of a religious holy day.

Q Drop Policy:

[If you want to drop a class after the 12th class day, you’ll need to execute a Q drop before the Q-drop deadline, which typically occurs near the middle of the semester. Under Texas law, you are only allowed six Q drops while you are in college at any public Texas institution. For more information, see: http://www.utexas.edu/ugs/csacc/academic/adddrop/qdrop]

Student Accommodations:

Students with a documented disability may request appropriate academic accommodations from the Division of Diversity and Community Engagement, Services for Students with Disabilities, 512-471-6259 (voice) or 1-866-329-3986 (video phone). http://ddce.utexas.edu/disability/about/

- Please request a meeting as soon as possible to discuss any accommodations
- Please notify me as soon as possible if the material being presented in class is not accessible
- Please notify me if any of the physical space is difficult for you

Academic Integrity:

Each student in the course is expected to abide by the University of Texas Honor Code:

“As a student of The University of Texas at Austin, I shall abide by the core values of the University and uphold academic integrity.”

You are responsible for understanding UT’s Academic Honesty Policy which can be found at the following web address: http://deanofstudents.utexas.edu/sjs/acint_student.php

University Electronic Mail Notification Policy
(Use of E-mail for Official Correspondence to Students):

Electronic mail (email), like postal mail, is a mechanism for official University communication to students. The University will exercise the right to send email communications to all students, and the University will expect that email communications will be received and read in a timely manner. The complete text of this policy and instructions for updating your e-mail address are available at http://www.utexas.edu/its/policies/emailnotify.html
Counseling and Mental Health Center:

The Counseling and Mental Health Center (CMHC) provides counseling, psychiatric, consultation, and prevention services that facilitate students’ academic and life goals and enhance their personal growth and well-being. [https://cmhc.utexas.edu](https://cmhc.utexas.edu)

Student Emergency Services:

Student Emergency Services supports students through challenging or unexpected situations by providing outreach, advocacy, intervention, and referrals to relevant campus and community organizations. [http://deanofstudents.utexas.edu/emergency/](http://deanofstudents.utexas.edu/emergency/)

The University Writing Center:

The University Writing Center offers free, individualized, expert help with writing for any UT student, by appointment or on a drop-in basis. Consultants help students develop strategies to improve their writing. The assistance we provide is intended to foster students’ resourcefulness and self-reliance. [http://uwc.utexas.edu/](http://uwc.utexas.edu/)

BCAL – Behavior Concerns Advice Line:

If you have concerns about the safety or behavior of fellow students, TAs or Professors, call BCAL (the Behavior Concerns Advice Line): 512-232-5050. Your call can be anonymous. If something doesn’t feel right – it probably isn’t. Trust your instincts and share your concerns.

Evacuation Information:

The following recommendations regarding emergency evacuation from the Office of Campus Safety and Security, 512-471-5767, [http://www.utexas.edu/safety/](http://www.utexas.edu/safety/)

Occupants of buildings on The University of Texas at Austin campus are required to evacuate buildings when an alarm or alert is activated. Alarm activation or announcement requires exiting and assembling outside, unless told otherwise by an official representative.

- Familiarize yourself with all exit doors of each classroom and building you may occupy. Remember that the nearest exit door may not be the one you used when entering the building.
- Students requiring assistance in evacuation shall inform their instructor in writing during the first week of class.
- In the event of an evacuation, follow the instruction of faculty or class instructors. Do not re-enter a building unless given instructions by the following: Austin Fire Department, The University of Texas at Austin Police Department, or Fire Prevention Services office.

Link to information regarding emergency evacuation routes and emergency procedures can be found at: [www.utexas.edu/emergency](http://www.utexas.edu/emergency)