**Introduction to Computational Materials Science**

**Instructor: Ye Cao**

**Office Number: ELB 334**

**Office Telephone Number:** 817-272-1858

**Email Address: ye.cao@uta.edu**

**Faculty Profile:** https://mentis.uta.edu/explore/profile/ye-cao

**Office Hours:** Thursday 3:30am-4:30pm

**Section Information:** MSE 5390-006, 4390-006

**Time and Place of Class Meetings:** Tuesday and Thursday 2:00-3:20pm, ELAB 256 (Computer Lab)

**Description of Course Content:** This course provides fundamentals of computational materials sciences, such as molecular dynamics, first-principles calculation, density functional theory and phase-field simulation. This course will also provide students with hands-on experience using different materials simulation method including XMD, Quantum Espresso, VASP and phase-field modeling to study different problems such as energy calculation, melting and sintering, vacancy diffusion and phase transition.

**Student Learning Outcomes:** Students become familiar with fundamental computational methods for different problems at different temporal and length scale, and better understand fundamental kinetic behaviors in materials science from computational perspective. Students will also get familiar with basic Linux commands.

**Required Textbooks and Other Course Materials:**
"Introduction to Computational Materials Science --- Fundamentals to Applications" by Richard Lesar
"Computational Materials Science --- An Introduction" 2nd edition by June Gunn Lee

**Descriptions of major assignments and examinations:**
There will be eight homework during the course, one final project and in-class presentation.

**Attendance:**
Attendance is required. If a student misses more than three lectures, she/he cannot get an A final grade.

**Grading**:

| | |
|---|---|
| Homework | 60% |
| Final Project and Presentation | 40% |

**Drop Policy:**
Students may drop or swap (adding and dropping a class concurrently) classes through self-service in MyMav from the beginning of the registration period through the late registration period. After the late registration period, students must see their academic advisor to drop a class or withdraw. Drops can continue through a point two-thirds of the way through the term or session. It is the student's responsibility to officially withdraw if they do not plan to attend after registering. **Students will not be automatically dropped for non-attendance**. Repayment of certain types of financial aid administered through the University may be required as the result of dropping classes or withdrawing. For more information, contact the Office of Financial Aid and Scholarships (http://wweb.uta.edu/aao/fao/).

**Americans with Disabilities Act:** The University of Texas at Arlington is on record as being committed to both the spirit and letter of all federal equal opportunity legislation, including the *Americans with Disabilities Act (ADA)*. All instructors at UT Arlington are required by law to provide "reasonable

accommodations" to students with disabilities, so as not to discriminate on the basis of that disability. Any student requiring an accommodation for this course must provide the instructor with official documentation in the form of a letter certified by the staff in the Office for Students with Disabilities, University Hall 102. Only those students who have officially documented a need for an accommodation will have their request honored. Information regarding diagnostic criteria and policies for obtaining disability-based academic accommodations can be found at www.uta.edu/disability or by calling the Office for Students with Disabilities at (817) 272-3364.

**Academic Integrity:** Students enrolled in this course are expected to adhere to the UT Arlington Honor Code:

> *I pledge, on my honor, to uphold UT Arlington's tradition of academic integrity, a tradition that values hard work and honest effort in the pursuit of academic excellence.*
>
> *I promise that I will submit only work that I personally create or contribute to group collaborations, and I will appropriately reference any work from other sources. I will follow the highest standards of integrity and uphold the spirit of the Honor Code.*

UT Arlington faculty members may employ the Honor Code as they see fit in their courses, including (but not limited to) having students acknowledge the honor code as part of an examination or requiring students to incorporate the honor code into any work submitted. Per UT System *Regents' Rule* 50101, §2.2, suspected violations of university's standards for academic integrity (including the Honor Code) will be referred to the Office of Student Conduct. Violators will be disciplined in accordance with University policy, which may result in the student's suspension or expulsion from the University.

**Student Support Services**: UT Arlington provides a variety of resources and programs designed to help students develop academic skills, deal with personal situations, and better understand concepts and information related to their courses. Resources include tutoring, major-based learning centers, developmental education, advising and mentoring, personal counseling, and federally funded programs. For individualized referrals, students may visit the reception desk at University College (Ransom Hall), call the Maverick Resource Hotline at 817-272-6107, send a message to resources@uta.edu, or view the information at www.uta.edu/resources.

**Electronic Communication:** UT Arlington has adopted MavMail as its official means to communicate with students about important deadlines and events, as well as to transact university-related business regarding financial aid, tuition, grades, graduation, etc. All students are assigned a MavMail account and are responsible for checking the inbox regularly. There is no additional charge to students for using this account, which remains active even after graduation. Information about activating and using MavMail is available at http://www.uta.edu/oit/cs/email/mavmail.php.

**Student Feedback Survey:** At the end of each term, students enrolled in classes categorized as "lecture," "seminar," or "laboratory" shall be directed to complete an online Student Feedback Survey (SFS). Instructions on how to access the SFS for this course will be sent directly to each student through MavMail approximately 10 days before the end of the term. Each student's feedback enters the SFS database anonymously and is aggregated with that of other students enrolled in the course. UT Arlington's effort to solicit, gather, tabulate, and publish student feedback is required by state law; students are strongly urged to participate. For more information, visit http://www.uta.edu/sfs.

**Final Review Week:** A period of five class days prior to the first day of final examinations in the long sessions shall be designated as Final Review Week. The purpose of this week is to allow students sufficient time to prepare for final examinations. During this week, there shall be no scheduled activities such as required field trips or performances; and no instructor shall assign any themes, research problems or exercises of similar scope that have a completion date during or following this week *unless specified in the class syllabus*. During Final Review Week, an instructor shall not give any examinations constituting 10% or more of the final grade, except makeup tests and laboratory examinations. In addition, no instructor shall give any portion of the final examination during Final Review Week. During this week,

classes are held as scheduled. In addition, instructors are not required to limit content to topics that have been previously covered; they may introduce new concepts as appropriate.

**Emergency Exit Procedures:** Should we experience an emergency event that requires us to vacate the building, students should exit the room and move toward the nearest exit. When exiting the building during an emergency, one should never take an elevator but should use the stairwells. Faculty members and instructional staff will assist students in selecting the safest route for evacuation and will make arrangements to assist handicapped individuals.

## Course Schedule (tentative):

| Lecture | Date | Subject |
|---|---|---|
| 1 | 01/16 | Introduction to computational materials sciences |
| 2 | 01/18 | The random-walk model |
| 3 | 01/23 | The random-walk model |
| 4 | 01/25 | Molecular dynamics |
| 5 | 01/30 | Molecular dynamics |
| 6 | 02/01 | Molecular dynamics |
| 7 | 02/06 | Molecular dynamics |
| 8 | 02/08 | Molecular dynamics |
| 9 | 02/13 | Molecular dynamics |
| 10 | 02/15 | Molecular dynamics |
| 11 | 02/20 | Molecular dynamics |
| 12 | 02/22 | First-principles methods |
| 13 | 02/27 | First-principles methods |
| 14 | 03/01 | First-principles methods |
| 15 | 03/06 | First-principles methods |
| 16 | 03/08 | First-principles methods |
| 17 | 03/20 | Density functional theory |
| 18 | 03/22 | Density functional theory |
| 19 | 03/27 | Density functional theory |
| 20 | 03/29 | Density functional theory |
| 21 | 04/03 | Density functional theory |
| 22 | 04/05 | Phase-field method |
| 23 | 04/10 | Phase-field method |
| 24 | 04/12 | Phase-field method |
| 25 | 04/17 | Phase-field method |
| 26 | 04/19 | Phase-field method |
| 27 | 04/24 | Phase-field method |
| 28 | 04/26 | Materials design and materials informatics |
| 29 | 05/01 | In-class presentation |
| 30 | 05/03 | In-class presentation |

* Guest lecturers may be invited

*"As the instructor for this course, I reserve the right to adjust this schedule in any way that serves the educational needs of the students enrolled in this course. –Ye Cao."*