COURSE SYLLABUS

ME-5329 - Computational Modeling for Engineering Systems – Fall 2025

Lecture Schedule: Tue, Thu 9:30 – 10:50 am (attendance mandatory)

Instructor:
Dr. Adelia Aquino
Office: MEN - 205
Email: adelia.aquino@ttu.edu

Office Hours: Tue, Thu 5:00 - 6:00 pm MEN 205
(or by appointment)

Prerequisite: None

Course Description:

This course covers the theory and application of modeling and simulation approaches including quantum-mechanical electronic structure methods (such as density-functional theory), classical force fields, and molecular dynamics. The electronic structure and molecular dynamics simulation methods are tools that can be used in the prediction of i) chemical reaction mechanisms such as combustion reactions as well as ii) the functional material properties for example elastic constants, Young's modulus, thermodynamics properties, color, and other properties directly from the chemical composition of the material based on quantum mechanics to solve Schroedinger's equation. This course will provide students with a practical understanding of both the fundamentals and applications of the above-mentioned methods to key engineering (nanotechnology and energy) problems.

Recommended Texts:

Frank Jensen, Introduction to Computational Chemistry, 3rd Edition, John Wiley & Sons, 2017
June Gunn Lee, Computational Materials Science, An Introduction, 2nd Edition, CRC Press, Taylor & Francis Group, 2017.
Daan Frenkel and Berend Smit - Understanding Molecular Simulations: From Algorithms to Applications, 2nd Edition, Academic Press, 2001.
Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edition, Wiley, 2004.

Course Content:

- Schroedinger equation for electrons, Born-Oppenheimer approximation, basis set.
- Hartree-Fock (HF) and post-HF wavefunction based techniques.
- Density functional theory (DFT).
- Thermodynamic Parameters: Enthalpy, and Gibbs Free Energy.
- Mechanical Parameters: elastic constants, Young's modulus, and shear modulus.
- Electronic Properties: density of states (DOS), natural bond orbitals (NBO), and charge.
- Vibrational (infrared) spectroscopy for molecules and solids.
- Adsorption and exchange mechanisms involving combustion reactions between mineral surfaces (Al_2O_3) and different oxidizers.
- Introduction to Linux and the use of HPCC computers.

- How to use Python scripts to generate geometry calculation inputs.
- Computational chemistry of molecules and solids. The following computational codes will be used for electronic and dynamics calculations at ab initio level of theory in molecules: Gaussian and Orca. VASP and Quantum Expresso program suites will be taken for molecular dynamics and electronic computations in solids.
- Classical molecular mechanics, force fields (FF), for dynamics calculations the LAMMPS program will be used.

Important dates: August 25^{th} - Classes Begin
Nov 3^{rd} - Advance Registration Begins
Nov 17^{th} - Last Day to Declare Pass/Fail Intentions
Nov 26^{th} -30^{th} – Thanksgiving Vacation
Dec 3^{rd} – Last Day of Class

Supplies: Laptop

Outcome: After completing this course, the fully successful student will be able to understand the methods, capabilities, and limitations of molecular simulation. The students should be able to: i) make a sound choice regarding the quality of molecular simulation studies available in the literature; ii) decide if molecular simulation fits for application to their own research problem. If yes, choose the computational applicable to the specific subject; iii) understand the workings and limitations of commercial molecular simulation software. Additionally, it is expected that students be able to explain the concepts of Schrodinger equation, basis set, Born-Oppenheimer approximation and other relevant concepts discussed in class, demonstrating a deeper understanding of the molecular basis of physical behavior.

Assessment:

homework: Will be assigned at the end of each topic discussed in class.
midterms: There will be five projects held during the semester. Students will have five days to deliver each project.
final exam: Final project at the end of the semester, covering the final material that was presented in class. Students will have five days to deliver this project.
grading: For each homework, midterm, and final exam, you will receive a numerical score. These scores will be weighted as follows,

Homework	25%
Midterms	50%
Final Exam	25%

Relevant Texas Tech policies can be found here:

https://www.depts.ttu.edu/tlpdc/RequiredSyllabusStatements.php
https://www.depts.ttu.edu/tlpdc/RecommendedSyllabusStatements.php

AI use encouraged:

You are welcome to use generative artificial intelligence (AI) tools (such as ChatGPT) in this class as doing so aligns with our course learning goals. You are responsible for the information you submit based on an AI query and for assuring that it does not contain misinformation or unethical content and that it does not violate intellectual property laws. Your use of AI tools must be properly documented and cited appropriately for academic integrity.

AI use allowed with disclosure and citation:
You are permitted to use ChatGPT and other artificial intelligence (AI) tools to assist you in gathering information and brainstorming ideas but you may not copy and paste information directly from the AI tool and present it as your own without citation. You are responsible for the information you submit based on an AI query and for assuring that it does not contain misinformation or unethical content and that it does not violate intellectual property laws. Your use of AI tools must be properly documented and cited appropriately for academic integrity. You are expected to include a disclosure statement at the end of your assignment describing which AI tool you used and how you used it. For example, "ChatGPT was used to draft about 50 percent of this paper and to provide revision assistance. AI-produced content was edited for accuracy.

Safety and Wellness

The Texas Tech University (TTU) and Edward E. Whitacre Jr. College of Engineering are committed to the safety and wellness of our students by providing various services and resources.
Make sure you register with Tech Alert to get emergency notifications by phone call, text, or email. You are encouraged to review the Emergency Action Plans (EAPs) and watch the videos of Know What To Do In Emergency Events and Surviving an Active Shooter Event Training to be prepared for those emergency situations. Additionally, due to the nature of laboratory or design courses, it is mandatory for you to follow the university safety policies and any additional safety protocols required by the course instructor(s).
For your well-being, various services are available at the Student Counseling Center and Student Health Services. The Student Wellness Center provides convenient walk-in services M-F from 8 AM to 5 PM. Furthermore, the Texas Tech Crisis HelpLine (806-742-5555) provides 24/7/365 assistance for students experiencing a crisis or distress.

Emergency/Crisis Phone Number

TTU Police (UPD) Emergency	911
TTU Police (UPD) Non-Emergency	806.742.3931
TTU Emergency Maintenance	806.742.4OPS (4677)

TTU EHS (M-F, 8 am – 5 pm)	806.742.3876
SafeRide	806.742.RIDE (7433)
TTU Crisis HelpLine	806.742.5555
Student Wellness Center (From Urgent Care to a Full-Service Pharmacy on site)	806.742.2848
Title IX Reporting	806.742.7233
The Dean of Students	806.742.2984