Course number and name

MTSE 4040 – Computational Materials Science

Credits and contact hours

3 Credits. Walk in or by appointment

Instructor's or course coordinator's name

Instructor: Zhenhai Xia

Text book, title, author, and year

No text book required. Lecture notes and class projects will be provided as handouts.

a. *Other supplemental materials*
   None

Specific Course Information

a. *Brief description of the content of the course (catalog description)*

   Introduction to the basic principles used to simulate, model and visualize the structure and properties of materials. Topics include various methods used at different length and time scales ranging from atomistic to the macroscopic.

b. *Prerequisites or co-requisites*

   MTSE3100, MTSE3030, MATH3310.

c. *Indicate whether a required, elective, or selected elective course in the program*

   Elective

Specific goals for the course

a. *Specific outcomes of instruction*

   - Introduce students to materials modeling and simulation techniques, such as density function theory (DFT), molecular dynamics (MD), and finite element method (FEM), that cover a wide time and length scales.
   - Show how these modeling methods can be used to understand fundamental material structure, material defects and the relationships between material structure and material behavior.
   - Develop an understanding of the assumptions and approximations that are involved in the modeling frameworks at the various time and length scales.

b. *Explicitly indicate which of the student outcomes listed in Criterion 3 or any other outcomes are addressed by the course.*

This course addresses ABET Criterion 3 Student Outcome(s): 1, 6,7 and Program Outcomes 1, 3, 4, 5, 7, 11.

4040: Computational Materials Science

Student/ABET Outcome	1	2	3	4	5	6	7
Specific Course Learning Outcome	x					x	x
1. Introduce students to materials modeling and simulation techniques, such as density function theory (DFT), molecular dynamics (MD), dislocation dynamics (DD) and finite element method (FEM), that cover a wide time and length scales.	x					x	x
2. Show how these modeling methods can be used to understand fundamental material structure, material defects and the relationships between material structure and material behavior.	x					x	x
3. Develop an understanding of the assumptions and approximations that are involved in the modeling frameworks at the various time and length scales.	x					x	x

Brief list of topics to be covered

1. Introduction and overview
2. Introduction to quantum mechanical modeling: Hartree-Fock and Density Functional Theory
3. Plane wave based DFT calculations
4. Quantum mechanics project: equilibrium properties and surfaces from DFT calculations
5. Atomistic modeling of defects in materials.
6. Molecular dynamics and Monte Carlo methods
7. Atomistic simulation project
8. Introduction to continuum mechanics and elasticity
9. Continuum mechanics and the finite element method
10. Finite element simulation project