

COMPUTATIONAL MATERIALS (CMPMT)

CMPMT 419: Computational Materials Science and Engineering

3 Credits

Introduction to computational material science and engineering. Overview of the computational methods for materials, from atomistic to the continuum scale. MATSE 419 Computational Materials Science and Engineering (3) Modeling is a critically important tool in the field of materials. This course is designed to inform students about all areas of materials modeling, and to explore the use of modeling in different research areas. This is a hands-on undergraduate level course, mandatory for all MATSE students, covering current methods for modeling soft and hard matter, at the atomistic, meso and continuum scale levels. It consists of an overview of individual techniques of modeling from atomistic molecular dynamics and Monte Carlo, coarse-grained molecular dynamics, and multiscale modeling, to the continuum (e.g. SAFT, CALPHAD). It also includes a computer laboratory component with hands-on exercises. At the conclusion of the course, students will understand the physical basis and basic procedures of each technique. Students will be able to understand the general literature in modeling and its connection with experimental work, as well as to communicate with experts in the field. From the laboratory practices, they will learn how the individual modeling techniques contribute to knowledge in each area, and to interconnect them with experimental information.

Prerequisite: CMPSC 200 and MATSE 201 and MATSE 202 and MATH 220 and (MATH 231 or MATH 230) and MATH 251
Cross-listed with: MATSE 419