

The 3rd IIMEC School on Computational Materials Science will take place on the Texas A&M University campus in College Station, Texas. The school is organized by the International Institute on Multifunctional Materials for Energy Conversion (IIMEC) and participating US institutions (Texas A&M University, University of Houston, Penn State) as well as international partners.

Purpose: To provide a platform for knowledge exchange and for academics as well as training for graduate students interested in the area of Computational Materials Science across multiple scales of space and time.

Objectives: At the end of this course, attendees should have a thorough overview of some of the most important tools currently in use to investigate materials phenomena at multiple scales, ranging from the continuum to the electronic structure level.

Structure: The School is organized in thematic sessions focused on different computational techniques. The themes will be organized in a top-down manner, starting with simulation tools at the continuum level, and finalizing the course with an overview of techniques that investigate materials at the electronic structure levels. The course duration will be 10 days. Morning sessions will consist of an overview of the method, with the afternoon sessions dedicated to hands-on computational laboratory activities.

Who should attend: The course should appeal to graduate students in the broader field of materials science with an interest in learning more about computational materials science.

Organization and Topics:

Themes will be organized as follows:

1. Atomistic Simulation
2. Thermodynamics and Kinetics of Materials at the Mesoscale
3. Microstructural Evolution
4. Mesoscale Phenomena
5. Continuum Response of Microstructures
6. General Approaches for Multi-Physics Modeling
7. Tool integration
8. Computer-Aided Materials Design

The School will consist of theoretical modules offered by experts in the field, followed by practical laboratories where the participants will have the opportunity of using the methods reviewed to simulate specific material phenomena. The computational resources available to the IIMEC collaboration as well as the recent Supercomputing Facilities acquired by Texas A&M University will be available for the instruction and practice sessions.

Interactions among participants is fundamental to achieve the full potential of the Winter School and social activities will be planned to provide ample opportunity to exchange experiences and ideas as well as to initiate collaborations that can be fostered within the IIMEC program.

Hardware/Software Available

During the Summer School, students and instructors will have access to a Linux Cluster consisting several hundred nodes/cores. State-of-the-art computational codes such as Thermo-Calc, FiPy, VASP, ABAQUS, LAMMPS, MATLAB will be used to illustrate the concepts covered in the school.