ATOMISTIC SIMULATION OF MATERIALS

Syllabus

Course Topic:
Atomistic Simulation of Materials

Number of Credits
5 ECTS

Course Responsible:
Tel Aviv University
Department of Materials Science and Engineering
Dr Oswaldo Diéguez

Course Lecturer:
Dr Oswaldo Diéguez

Prerequisites:
Previous exposure to a university course in general physics or general chemistry. Previous exposure to computer programming in any language.

Learning Outcomes:
Upon completion of this course the student will be able to:

- Explain the basic physical theories behind the most used models to do atomistic simulations of materials (e.g., classical semiempirical potentials and quantum-mechanical density-functional theory).
- Implement those models in a computer language of choice to produce software for numerical calculations.
- Carry out numerical experiments that rely on atomistic models for materials.
- Perform analysis of those numerical experiments in order to gain understanding about the properties of particular materials.
- Critically read the scientific literature presenting results obtained using atomistic simulation of materials.

Abstract:
All materials are made of atoms. This simple and powerful statement will serve as the scientific basis of this course. We will model the interaction between atoms or their parts using different methods. We will implement these models into computer programs for doing numerical experiments. Then, we will analyze the results of these numerical experiments to gain understanding about the macroscopic properties of materials: their structure, vibrational properties, electronic properties, and more.

Content:

1. Introduction to Atomistic Simulation of Materials: Review of Classical Mechanics, Quantum Mechanics, Statistical Mechanics, and Computers.
2. Monte Carlo Methods: The Example of a Phase Transition in a Hard Spheres System.
3. Molecular Dynamics: The Example of a Phase Transition in a Hard Spheres System.
4. Interatomic Potentials: Computing Properties of Materials using Molecular Dynamics.
5. Quantum Mechanics: The Example of the Hydrogen Molecule.
6. Tight Binding Method for Carbon: Implementation and Computation of the Properties of Diamond and Graphite.
7. First-Principles Methods: The Example of the Siesta Code to Study Molecules, Insulators, and Metals.
8. Atomistic Simulation of Materials Today.

Teaching Methods:
Each unit of the course contains explanations about the concepts to be covered, and a small research project that requires application of these concepts. The explanations will be recorded in short videos, where the instructor will describe the main physical concepts relevant to the unit. Then, the student will download a report with a description of a small computational project, where understanding of the topic will be needed to carry out some numerical experiments. This report will contain enough information so that the student can check that his/her code implementation is correct, and whether the results of the numerical experiments will make sense.

Assessment:
50% of the grade will come from practical work of the students in exercises that require writing scientific code and performing numerical experiments. 50% of the grade will come from a multiple-choice test about the concepts learned in the course.

Recommended Reading:
We will use several articles from the scientific literature of atomistic simulation of materials. In addition, the following books can be helpful in learning some of the concepts in the course:

- *Computational Physics*, by Thijssen, Cambridge University Press (1999).
- *Computer Simulation of Liquids*, by Allen and Tildesley, Oxford University Press (1989).
- *Electronic Structure: Basic Theory and Applications*, by Martin, Cambridge University Press (2008).
- *Molecular Dynamics Simulation: Elementary Methods*, by Haile, Wiley-Interscience (1997).
- *Understanding Molecular Simulation: From Algorithms to Applications*, by Frenkel, Academic Press (2001).