Full Syllabus

Course Title

Introduction to Computational Materials Science

Lecturer

Prof Oswaldo Dieguez (TA: Netanela Cohen)

Semester

Bet

Course requirements

Any course on programming (for example, 0509.1820 Programming in Python)

Final grade components

5% Lecture on-Campus Attendance, 20% Homework, 75% Final Exam (multiple-choice test).

Course schedule

Class no. / Date	Subject and Requirements (assignments, reading materials, tasks, etc.)
1	Introduction to the Course
2	The Random Walk Model I
3	The Random Walk Model II
4	Simulation of Atomic Systems I
5	Simulation of Atomic Systems II
6	Molecular Dynamics I
7	Molecular Dynamics II
8	The Monte Carlo Method I
9	The Monte Carlo Method II
10	Molecular and Macromolecular Systems
11	Kinetic Monte Carlo I
12	Kinetic Monte Carlo II
13	Review

Required course reading

None

Optional course reading

The Topics of the Course are discussed in:
• Introduction to Computational Materials Science: Fundamentals to Applications, by Richard LeSar, Cambridge University Press (2013).
Other books that cover some of the topics of the course (on a more advanced level) are:
• Computer Simulation of Liquids, by M.P. Allen and D.J. Tildesley, Oxford Science Publications (1989).
• Computational materials science: the simulation of materials microstructures and properties, by D. Raabe, Wiley (1998).
• Understanding Molecular Simulation: From Algorithms to Applications, by D. Frenkel and B. Smit, Academic Press (2001).
• The Art of Molecular Dynamics Simulation, by D.C. Rapaport, Cambridge University Press (2004).
• Modeling Materials: Continuum, Atomistic and Multiscale Techniques, by E. B. Tadmor and R.E. Miller, Cambridge University Press (2011).

Comments

Lectures will be delivered in person on Campus and streamed on zoom. Recordings will be made available.