TEL AVIV UNIVERSITY אוניברסיטת תל אביב

Full Syllabus

Course Title

Introduction to Computational Materials Science

Lecturer

Dr Oswaldo Dieguez (TA: Netanela Cohen)

Semester

Bet

Course requirements

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

Final grade components

25% Lecture Attendance, 25% Homework, 50% Exam (multiple-choice test).
Homework is due every week (no late submission is accepted). If you get a higher grade in the Exam than in the Homework, your final grade will be the one of the Exam.

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 on Campus if allowed; otherwise through zoom. Recordings will be made available.

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