TEL AVIV UNIVERSITY אוניברסיטת תל אביב

Course Title

Atomistic Simulation of Materials (0581-5221)

Lecturer

Prof Oswaldo Diéguez (dieguez@tau.ac.il)

Semester

1/2025

Course requirements

This is a **graduate** course designed for a materials science and engineering degree. It is expected that you have been exposed to beginning-level university courses in **general physics, general chemistry, quantum mechanics, mathematics, and at least one programming language** (we will be programming mainly in Fortran, but if you have taken a course in any other language, that will be enough to understand what we will do: Python, Matlab, C, Java, or any other similar one is good). **Do not** take this course if you are not comfortable with **one** programming language at least.

You will need a laptop in which you install software for the Course. **Please bring the laptop to class.**

Final grade components

Homework: There are weekly Homework assignments, which include mostly programming in Fortran and running your code and other codes available on the internet; **the Homework is demanding**, and it can take many hours per week if you have little experience with a computer language; your "Homework grade" is the average of your ten best weekly Homework grades.

Attendance: Attendance to class is not mandatory, but you get 10 points per lecture in which you are in class (no points for remote attendance).

FINAL GRADE: If your Homework grade is higher than your attendance grade, your final grade is your Homework grade; otherwise it is 90% of your Homework grade and 10% of your Attendance grade.

Course schedule

Class no. / Date	Subject and Requirements (assignments, reading materials, tasks, etc.)
1	*Introduction to the Course.*
2	*Molecular Dynamics of a Hard Sphere System I*
3	*Molecular Dynamics of a Hard Sphere System II*
4	*Molecular Dynamics of a Hard Sphere System III*
5	*Molecular Dynamics of a Hard Sphere System IV*
6	*Molecular Dynamics of a Hard Sphere System V*
7	*Molecular Dynamics of a Hard Sphere System VI*

8	*Learning About Materials with Siesta I.*
9	*Learning About Materials with Siesta II.*
10	*Learning About Materials with Siesta III.*
11	*Learning About Materials with Siesta IV.*
12	*Learning About Materials with Siesta V.*
13	*REVIEW.*

Required course reading

There is no required reading.

Optional course reading

No textbook is needed. Those students interested in learning more, or in alternative references to the work done in class, are welcome to consult the following:

- 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).

Comments

This Course is taught in English.

The Course will be taught on Campus. **Please bring your laptop to class.**

Reasonable attempts will be made to stream and record the lectures, but no guarantees are given. Please come to class.

The material of this Course will be available in the Moodle page of the Course:
https://moodle.tau.ac.il/course/view.php?id=581522101