Full Syllabus

Course Title

Atomistic Simulation of Materials

Lecturer

Dr Oswaldo Diéguez

Semester

1/2020

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).

Final grade components

100% Homework (your final grade will be the average of your weekly Homework assignments, which will include mostly programming in Fortran and running your and others' codes; the Homework is demanding, and it can take several hours per week if you have no previous experience with a computer language).

Course schedule

Class no. / Date	Subject and Requirements (assignments, reading materials, tasks, etc.)
1	*Overview of the Course. Introduction to the Hard Spheres Project.*
2	*Introduction to Fortran.*
3	*Designing and Implementing your Molecular Dynamics Code I.*
4	*Designing and Implementing your Molecular Dynamics Code II.*
5	*Designing and Implementing your Molecular Dynamics Code III.*
6	*Overview of Quantum Atoms. Introduction to the Tight-Binding Project.*
7	*Designing and Implementing your Tight-Binding Code I.*
8	*Designing and Implementing your Tight-Binding Code II.*
9	*Designing and Implementing your Tight-Binding Code III.*
10	*Overview of Density-Functional Theory. Introduction to the Siesta Project.*
11	*Learning About Materials with Siesta I.*
12	*Learning About Materials with Siesta II.*
13	*SUMMARY.*

Required course reading

There is no required reading.

Optional course reading

No textbook is needed. The Course focuses in learning by implementing programs to do atomistic simulations, and all the details are worked out in class and with the help of scientific publications that will be available in the Moodle page of our Course. Those students interested in learning more, or in alternative references to the work done in class are welcome to consult these references:

- 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).

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Comments

This Course is taught in English.

In 2020/2021 the Course will be taught remotely through a combination of recorded videos on the topics and videoconferencing to answer questions you might have in real time. All the material of this Course (including links to those videos and to zoom virtual rooms) will be available in the Moodle page of the Course: https://moodle.tau.ac.il/course/view.php?id=581522101