MSE-305 **Introduction to atomic-scale modeling**

Ceriotti Michele

| Cursus | Sem. | Type |
|---|---|---|
| Auditeurs en ligne | E | Opt. |
| Materials Science and Engineering | BA6 | Obl. |

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| Language of teaching | English |
| Credits | 2 |
| Session | Summer |
| Semester | Spring |
| Exam | During the semester |
| Workload | 60h |
| Weeks | 14 |
| **Hours** | **2 weekly** |
| Courses | 2 weekly |
| **Number of positions** | |


## Summary

This course provides an introduction to the modeling of matter at the atomic scale, using interactive Jupyter notebooks to see several of the core concepts of materials science in action.


## Content

Simulation and modeling has become an integral part of the process of designing and optimizing materials for the most diverse applications. Truly predictive simulations, that can estimate the properties of materials before they have ever been synthesized, require atomistic resolution. This course provides an introduction to some of the techniques that underlie atomic-scale simulations of materials. With a strong hands-on component, based on interactive Jupyter notebooks, we will revisit, and see in a new light, several basic concepts on the nanometer-scale description of matter, and see a number of different modelling techniques in action, from molecular dynamics to atomic-scale machine learning.

## Keywords

materials modeling, computational thinking, Python, atomistic models

## Learning Prerequisites

### Required courses

The course requires a basic understanding of programming, such as that given in the first-year ICC course.

## Teaching methods

This course follows a "flipped class" format, and is based on a set of interactive Jupyter notebooks that contain "passive" demonstrations of materials-science concepts, short coding exercises that are aimed at developing both an intuition of the physical processes and some basic skills in using some simple tools for atomistic modeling, and open-ended questions that are graded during the course, but can also simply be used as a way to encourage reflection on the core concepts presented in each exercise.

## Expected student activities

The students will work individually on interactive jupyter notebooks, answering the questions and completing small coding assignments. While the bulk of the work will be performed during the lecture hours, and with the supervision of the teacher and TAs, in will often be necessary to complete the assignments at home.

## Assessment methods

The assignments will be graded during the term, and contribute 80% of the final grade. 20% of the grade will be assigned based on a short individual discussion with the teacher, at the end of the semester.

## Resources

### Moodle Link

- https://go.epfl.ch/MSE-305

### Videos

- https://mediaspace.epfl.ch/channel/MSE-305+Introduction+to+Atomic+Scale+Modeling/29408