EPFL

MSE-468	**Atomistic and quantum simulations of materials**
	Marzari Nicola

Cursus	Sem.	Type
Computational science and Engineering	MA2, MA4	Opt.
Materials Science and Engineering	MA2, MA4	Opt.

Language of teaching	English
Credits	4
Session	Summer
Semester	Spring
Exam	During the semester
Workload	120h
Weeks	14
Hours	**4 weekly**
Courses	2 weekly
TP	2 weekly
Number of positions	

Summary

Theory and application of quantum simulations to model, understand, and predict the properties of real materials.

Content

Materials simulations: classical and quantum models. Electronic-structure and first-principles approaches (density-functional theory and the total-energy pseudopotential method). Temperature and thermodynamic averages: Monte Carlo sampling and molecular dynamics simulations. How to obtain materials' properties from simulations. Computational laboratories: Mechanical properties of materials. Band structures and electrical transport. Molecular dynamics and diffusion coefficients. Phonons and vibrational spectroscopies.

Learning Prerequisites

Recommended courses

Fundamentals of solid-state materials, or similar.

Learning Outcomes

By the end of the course, the student must be able to:
- Model materials with quantum mechanical simulations

Teaching methods

Ex cathedra and computational laboratories

Assessment methods

Written reports of computational labs