

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
<b>Hours</b>	<b>4 weekly</b>
Courses	3 weekly
TP	1 weekly
<b>Number of positions</b>	

**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