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

Pizzi Giovanni

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	3 weekly
TP	1 weekly
Number of positions	

Summary

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

Content

- Materials simulations and energy models: from classical potentials to quantum models.
- Electronic-structure and first-principles approaches (density-functional theory and the total-energy pseudopotential method).
- Errors and accuracy of quantitative predictions.
- Temperature and thermodynamic averages: Monte Carlo sampling and molecular dynamics simulations.
- Free energies and phase transitions.
- How to obtain materials' properties from simulations.
- Computational laboratories: Mechanical properties of materials (classical and quantum approaches). Electronic band structures and density of states. Molecular dynamics, diffusion coefficients and phase transitions. These labs will be performed using well known simulation codes, like GULP (for the classical simulations) and Quantum ESPRESSO (for the quantum simulations).

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

Resources

Virtual desktop infrastructure (VDI)
Yes

Bibliography

General references

• Ellad Tadmor and Ronald Miller, “Modelling Materials” Cambridge University Press
• Rob Phillips, "Crystals, Defects and Microstructures", Cambridge University Press

Electronic-structure and DFT

• Feliciano Giustino, “Materials Modelling using Density Functional Theory”, Oxford University Press
• Richard Martin, “Electronic Structure”, Cambridge University Press
• Efthimios Kaxiras, “Atomic and Electronic Structure of Solids”, Cambridge University Press
• Jorge Kohanoff, “Electronic Structure Calculations for Solids and Molecules”, Cambridge University Press

Simulation codes

• Quantum ESPRESSO: https://www.quantum-espresso.org
• GULP: http://gulp.curtin.edu.au/gulp/

Ressources en bibliothèque

• Modeling Materials / Tadmor