

MSE-423 Fundamentals of solid-state materials

Marzari Nicola

Cursus	Sem.	Type
Materials Science and Engineering	MA1, MA3	Obl.

Language of **English** teaching Credits Session Winter Semester Fall Exam Oral Workload 120h Weeks 14 Hours 4 weekly 3 weekly Courses Exercises 1 weekly Number of positions

Summary

Fundamentals of quantum mechanics as applied to atoms, molecules, and solids. Electronic, optical, and magnetic properties of solids.

Content

Fundamentals of electronic structure: the Schroedinger equation and its solution for free electrons, electrons in a potential well, and in a Coulomb potential. Variational principle and diagonalization. Electronic structure of molecules, and approximate solutations with linear combination of atomic orbitals. Hartree-Fock. Symmetry operation and their role in classifying eigenstates. Hamiltonian in a periodic potential and energy bands. Free-electron and tight-binding models. Fermi-Dirac statistics and distribution. Electrical transport and semiconductors. Optical properties of materials, and their quantum origin. Magnetic properties of materials.

Learning Prerequisites

Required courses

Basic knowledge of classical mechanics and electromagnetism.

Learning Outcomes

• Elaborate the electronic origin of materials properties

Assessment methods

Oral exam