UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Advanced Solid State Physics

2425-1-FSM01Q021

Aims

The aims of this advanced course in Solid State Physics are to provide the conceptual tools and the notions that are particularly useful to the students undertaking a path in materials for digital technologies (ICT) and quantum technologies (QT). However, this course is also useful to students interested in materials for energy efficiency, such as the ones entering superconductive cables, LEDs and power-electronics devices.

Contents

Beyond the non-interacting electrons: many-electron theories, electronic screening, effects of a magnetic field, ferromagnetism, and superconductivity. Practical computational training based on Density Functional Theory for semiconducting materials and for magnetic materials, using the Vienna Ab-initio Simulation Package (VASP) or Quantum Espresso codes.

Detailed program

The many-electron problem and the effects of electronic screening

• From the many-electron system to the mean-field equation: Hartree equations
• The Hartree-Fock equations and meaning of the exchange energy contribution
• The interacting gas of free electrons
• Foundations of the density functional theory (DFT): the Hohenberg and Kohn theorems
• The Kohn-Sham equations
• Ground-state properties and elementary excitations
• The muffin tin potential and the augmented plane waves

- Orthogonalization of valence states to core states: orthogonalized plane waves and pseudopotentials
- Electronic screening in the Thomas-Fermi model
- Electronic screening in the perturbative, Lindhard model
- Bonding and crystal structure in simple metals and other solids

Density Functional Theory in practice

- What can DFT predict? Structural Properties, Cohesive/Formation/Surface energies, Electronic Properties, Vibrational properties, Optical properties
- Do we trust DFT? Precision and Accuracy
- Where is DFT failing? How to overcome failures?
- High-throughput simulations and browsing over DFT databases (i.e. MaterialsProject, MaterialsCloud, C2DB, …).

DFT Hands-on (I): Structural and Electronic Properties of GaAs Zincblende Semiconductor

- Getting used to Linux environment.
- Explanation of flags and info contained in input and output files of DFT codes.
- First simulation of a self-consistent cycle for zincblende GaAs.
- Convergence tests as a function of k-point grid in the Brillouin zone and energy cut-off.
- Calculation of equilibrium lattice constant of GaAs using the Birch-Murnaghan Equation of state and comparison with experiments.
- Band-structure calculations (I): construction of k-points path in reciprocal space along high-symmetry lines, non-self-consistent simulation of band-structure for GaAs and use of related plotting tools.
- Estimate of DFT band-gap and effective mass.
- Density of states (DOS): non-self-consistent simulation for GaAs of total DOS and DOS projected on atoms and orbitals.

Magnetic properties of solids

- Stoner model for band ferromagnetism in metallic solids
- Effect of temperature in the Stoner model, Curie temperature
- Ferromagnetism in insulating solids and the Heisenberg hamiltonian
- Antiferromagnetism and anisotropic magnetic susceptivity
- Excited magnetic states: spin waves and magnons
- Neutron scattering, role of magnons at low temperature
- Ferromagnetic domains

DFT Hands-on (II): DFT for magnetic systems

- DFT predictions for magnetic properties: literature overview
- DFT simulations for elemental magnetic solids.
- Use of Stoner criterium to predict the occurrence of magnetism: comparison of bcc-Fe with and without spin-polarization.
- Magnetostrictive effects: plot Energy vs Volume E(V) curve for magnetic and non-magnetic bcc-Fe.
- DFT for 2D magnets: i) Spin-orbit coupling and magnetic anisotropy energy. ii) Long-range magnetic ordering (including antiferromagnetism) and first-principles estimate of parameters in spin-Hamiltonian

Superconductivity

- Introduction to superconductivity: Onnes experiment and Meissner-Ochsenfeld effect
- The London and London equations: penetration of currents and magnetic fields
- The thermodynamics of the superconducting phase: free-energy, entropy and heat capacity
- Cooper pairs and instability of the Fermi sea
- Ground state in the Bardeen-Cooper-Schrieffer (BCS) theory
- Existence of the gap, its nature, and definition of the excited states in the BCS theory

• The supercurrent as steady state, critical values of current and magnetic field and Meissner effect in the BCS theory
• Experimental measurements of the gap, its temperature dependence and isotopic effect
• High-Tc superconductors

Prerequisites

Theory of infinite and periodic solids in the single-electron scheme (basic course in Solid State Physics). Quantum mechanics.

Teaching form

Lessons, practice lessons, and discussions with the students.

- 16 front-lessons (2 hours each) in presence (32 h in total);
- 4 computational lab activities (4 hours each) in presence (16 h in total);
- 4 computational lab activities (2 hours each) remote (8 h in total).

Textbook and teaching resource

All the material which is strictly necessary to the exam is uploaded as .pdf presentations of the lessons in the e-learning platform.

MAIN TEXTBOOKS:

• H. IBACH AND H. LUTH, Solids State Physics, Fourth Edition, Springer Verlag 2009.
• N.W ASHCROFT AND N.D. MERMIN, Solid State Physics, Saunders College Publishing
• R. M. MARTIN, Electronic Structure: Basic Theory and Practical Methods, Cambridge University Press

ADDITIONAL TEXTS

• F. BASSANI E U. GRASSANO, Fisica dello Stato Solido, Casa Editrice Boringhieri
• G. GROSSO AND G. PASTORI PARRAVICINI, Solid state Physics, Academic Press
• S. BLUNDELL, Magnetism in Condensed Matter, Oxford University Press.
• M. L. COHEN & S. G. LOUIE, Fundamentals of Condensed Matter Physics, Cambridge University Press

Semester

Second Semester

Assessment method

Oral examination with three open questions, referring to different parts of the program. Short oral presentation focused on one of the DFT hands-on sessions. The mark is produced by an average of the three answers and of the discussion of the results of the simulations. No intermediate exams will be carried out.

Office hours

By e-mail appointment with the teacher

Sustainable Development Goals

QUALITY EDUCATION | INDUSTRY, INNOVATION AND INFRASTRUCTURE