COURSE SYLLABUS

Advanced Solid State Physics

2526-1-FSM02Q021

Aims

The aims of this course are: 1) knowledge and understanding: to facilitate learning and comprehension in some key areas of Solid State physics, such as materials modelling and quantum phenomena in hard condensed matter physics; 2) applying knowledge and understanding: to provide adequate tools to analyze complex phenomena from the fundamental point of view, by means of microscopic understanding and first-principles simulations; 3) making judgements: to help students develop a critical thinking in the analysis of materials properties, for example, on the basis of simulation results; 4) communication skills: to support students in learning how to interact with academic and research professionals in the field of solid state physics, i.e. by means of appropriate technical and scientific language, presentation tools and related skills; 5) learning skills: to master scientific and computational competences to enable students to critically analyze the scientific literature and engage with modern avenues of solid state physics.

Contents

Beyond the non-interacting electrons: many-electron theories, magnetism, 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).

Detailed program

The many-electron problem
• From the many-electron system to mean-field theories: Hartree equations
• The Hartree-Fock equations and the exchange energy contribution
• The homogeneous electron gas

• Foundations of density functional theory (DFT): the Hohenberg and Kohn theorems
• The Kohn-Sham equations
• Exchange-correlation functional and Local Density Approximation
• Pseudopotentials

Density Functional Theory in practice:
• What can DFT predict? Examples of relevant material properties obtained from first-principles
• Do we trust DFT? Precision and Accuracy
• Where is DFT failing? How to overcome failures?

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 vs k-point grid in the Brillouin zone and energy cut-off.
• Calculation of equilibrium lattice constant of GaAs 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 and use of related plotting tools.
• Estimate of DFT band-gap
• Density of states (DOS): non-self-consistent simulation for GaAs of total DOS and DOS projected on atoms and orbitals.

Magnetic properties of solids
• Introduction to Ferro-/Antiferro-/Para-magnetism
• Stoner model for band ferromagnetism in metallic solids
• Ferromagnetism in insulating solids and the Heisenberg hamiltonian
• Antiferromagnetism and neutron scattering
• Magnetic anisotropy
• Excited magnetic states: spin waves
• Magnetic 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 Ni-fcc with and without spin-polarization.
• DFT for 2D magnets: i) Long-range magnetic ordering (including antiferro-magnetism) and first-principles estimate of exchange parameters in spin-Hamiltonian ; i) Spin-orbit coupling and magnetic anisotropy energy.

Superconductivity
• Introduction to superconductivity: Onnes experiment, Meissner effect, isotope effect
• The London and London equations: penetration of currents and magnetic fields
• The thermodynamics of the superconducting phase
• Cooper pairs
• Introduction to Bardeen-Cooper-Schrieffer (BCS) theory
• Existence of the gap, its nature, and excited states in the BCS theory
• Introduction to Landau-Ginzburg theory: coherence length vs penetration depth
• Type II superconductors and vortex-state
• High-Tc superconductors

Prerequisites

Deep understanding of: theory of infinite and periodic solids in the single-electron scheme (basic course in Solid State Physics). Quantum mechanics. Atomic and Molecular Quantum Physics.

Teaching form

Lessons, practice lessons, and discussions with the students.

- 14 front-lessons (2 hours each)
- 2 lessons in remote (2 hours each)
- 12 computational lab activities (2 hours each) in presence

Textbook and teaching resource

All the material which is strictly necessary to the exam is uploaded as .pdf presentations of the lessons on the e-learning platform.
MAIN TEXTBOOKS:
• F. GIUSTINO, Materials Modelling using Density Functional Theory, Oxford University Press
• N.A. SPALDIN, Magnetic Materials, Cambridge University Press
• C.A. KITTEL, Introduction to Solid State Physics, Wiley
ADDITIONAL TEXTS
• R. M. MARTIN, Electronic Structure: Basic Theory and Practical Methods, Cambridge University Press
• R. TURTON, The Physics of Solids, Oxford University Press
• S. BLUNDELL, Magnetism in Condensed Matter, Oxford University Press.
• H. IBACH AND H. LUTH, Solids State Physics, Fourth Edition, Springer Verlag

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