Electronic structure theory

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ECTS credits: 6

Language of instruction: English

Examination: written project report (50%) plus oral presentation (50%)

Description:

The goal of this course is to introduce the main methods in electronic structure theory, which is at the heart of our present capability of understanding, predicting, and engineering materials properties based on accurate *in-silico* solutions of the many-body Schrödinger equation for electrons and their coupling with the lattice/structural degrees of freedom. We will follow a teaching/learning approach that combines detailed explanations of the underlying formalisms and approximations to solve the quantum many-body electron-ion problem and the introduction to their actual implementations in working computer codes. While the most theoretical part will be developed during frontal lectures (cours magistraux), the introduction to the usage of computer codes will be done through hands-on sessions and the realization of computer lab projects (TPs), carried out in teams of two-three students each. The theory will cover the density functional theory (DFT) for the solution of the electronic problem, the density functional perturbation theory (DFPT) for the calculation of the lattice vibrational properties. Methods beyond DFT will be presented in the last part of the theory lectures, to resolve properties of strongly correlated materials. A particular focus will be done on dynamical mean field theory (DMFT). We will briefly cover also GW and quantum Monte Carlo (QMC) methods. For the hands-on sessions and computer lab projects, we will employ Quantum Espresso and TRICS, as DFT and DMFT packages, respectively.

Plan of the course:

I DFT (8h) + hands-on sessions (4h)

II DFPT (6h) + hands-on sessions (2h)

III DMFT (8h) + hands-on sessions (4h)

IV Computer projects (20h)