Modul: Density Functional Theory: Fundamentals and Practice

Lehrveranstaltungsnummer: 4024121 / 4024122
Modulverantwortliche: Evers
Einordnung in Studiengang: Master Physik, Themenfeld/er: Theorie der Kondensierten Materie, Nano-Physik
Leistungspunkte: 8
Semesterwochenstunden: 4
Modulturnus: SS
Lehr- und Lernformen: Vorlesung 2 SWS; Evers
Übungen 2 SWS: Evers/N.N.
Lernziele: Understanding the fundamentals of modern DFT. Apply common DFT-packages for standard applications in quantum chemistry and condensed matter physics.
Voraussetzungen: quantum mechanics

Inhalt:
The fascination and also the technological potential of nanostructured materials derives largely from the fact that material and device properties can be very sensitive to atomistic details. Conversely, in order to understand experiments with such systems it is often very helpful, if not mandatory, to have available computer simulations and theoretical analysis tools that can describe and even predict how the system specific behavior is brought about by its individual atomistic or molecular structure. For this reason, the use of commercial or freeware software packages that offer such analysis tools is proliferating in theoretical as well as in experimental nanosciences.

By far the most important framework for such theoretical studies is the density functional theory (DFT). DFT owes its attractiveness and popularity to the fact that it offers a balanced trade off between numerical accuracy (molecular/crystal geometries, binding energies, band structures, work function, etc.) and the computational effort. However, what too often goes unnoticed is that the relative simplicity of DFT is deceptive. Up to now, one has to employ approximations in virtually all available DFT implementations (e.g. the "local density approximation", LDA) which are not controlled and therefore can lead to qualitatively completely incorrect results.

To meet these observations and developments, we offer a lecture course with exercises to students, PhD-students, postdocs and interested scientists from theory and experiment. The lecture will introduce into the basic ideas of DFT with an emphasis on where in practice things can go wrong due to uncontrolled approximations. Specific topics that we cover include

- The constituting equations: Hohenberg-Kohn equations and Levy's derivation
- Fundamental properties of DFT: exact results
- The Kohn-Sham-formulation of DFT
- Aproximate functionals: LDA, GGA's and the hybrids
- Defects in common functionals and their consequences: The derivative discontinuity
- Applications of DFT: workfunctions, band-structures, lattice vibrations etc.

Our exercises offer a tutorial introduction into major software packages, AIMS and TURBOMOLE, and corresponding pedagogical examples in hands-on sessions.

- getting started: data format and input for ab-initio packages
- total energies and structure relaxation
- electronic structure and wavefunctions
- vibrations

Lectures will be delivered in English upon request.

Literatur: Will be given in the lecture
Leistungsnachweis: Nachweis der erfolgreichen Teilnahme an Übungen u. Hausaufgaben für den Übungsschein.

Notenbildung: mündliche Prüfung. Schein wird als Eingangsbedingung nicht verlangt.