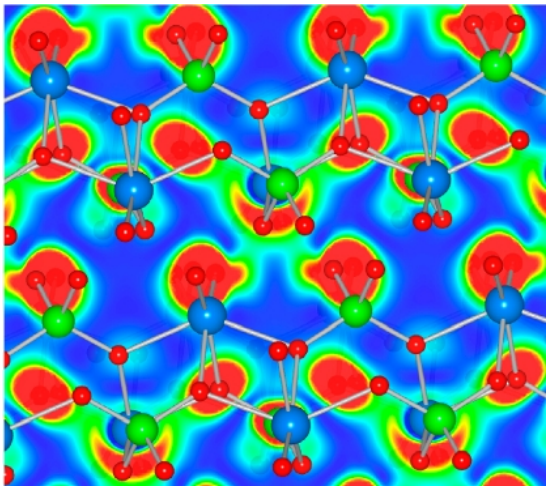
Density Functional Theory:

From Theory to Applications



Jun.-Prof. Dr. M. Sulpizi, WS 2010/11

Institut für Physik, Universität Mainz

Mondays **14.00-16.00** Seminarraum E **Bau 2/413, 01-231**

Begin:

Monday, 8. November 2010

The course will present an overview of Density Functional Theory, covering both theory and applications. The topics presented in the course include:

- **background** material on elementary quantum mechanics (Hartree Fock approximation, correlation energy, Hellmann-Feymann theorems);
- **modern Density functional Theory.** This will include Hoherberg-Kohn theorems, Thomas-Fermi theory, Kohn-Sham equations. Local Density Approximation, Spin Density Functional Theory;
- exchange correlation hole and reliability of LDA. Beyond LDA: the generalized gradient approximations, the hybrid functionals;
- ***ab initio* molecular dynamics:** Born-Oppenheimer molecular dynamics, Car-Parrinello dynamics and Ehrenfest dynamics;
- Basis set: plane wave and localized basis sets and pseudopotentials.
- **Applications of DFT**: From material to biomolecules. This would include: solids, liquids, interfaces. Biophysics and biochemistry: QM/MM techniques;
- **Properties** from ab initio molecular dynamics (IR, magnetism, NMR, EPR spectroscopy, redox properties);
- beyond the ground states: **time dependent DFT**. Photochemistry.