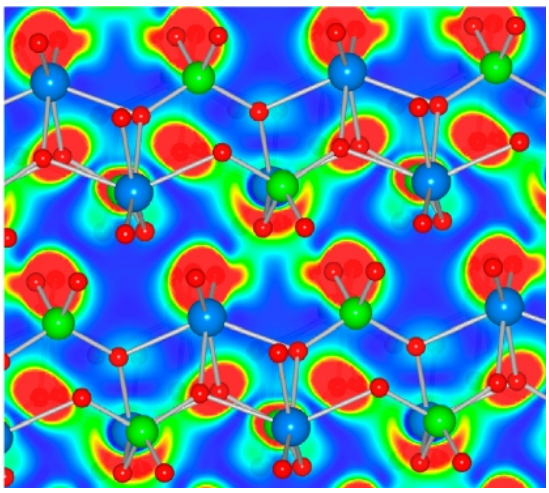
Density Functional Theory:

From Theory to Applications



Jun.-Prof. Dr. M. Sulpizi and Dr. Martin Oettel, WS 2011/12

Institut für Physik, Universität Mainz

Mo **14.00 (ST)-15.30;** Mi **12.00 (ST)-13.30;** Seminarraum E **Bau 2/413, 01-231**

Begin: Monday, 24. October 2011

The course will present an overview of Density Functional Theory, covering both theory and applications for classical statistical systems and quantum mechanics.

The topics presented in the course include:

Background and Foundation of Density Functional Theory:
Quantum mechanics: elementary quantum mechanics (Hartree Fock approximation, correlation energy, Hellmann-Feymann theorems); Hohenberg-Kohn theorems, Thomas-Fermi theory, Kohn-Sham equations. Local Density Approximation, Spin Density Functional Theory;
Classical statistical systems: review statistical mechanics (functional formulation); Hohenberg-Kohn theorems (Mermin version); comparison to quantum DFT
Further Elaborations and Applications:
Quantum Mechanics: 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.
Classical Statistical Systems: Nearly exactly solvable systems: Hard Bodies Perturbation strategies

If you are interested to come, but you cannot come on the first lecture, please send us an e-mail, so I can have an estimate of the numbers. For **more informations** please contact us at sulpizi@uni-mainz.de