FDITE210 Density Functional Theory

Lecturer: Dr. Gábor Paragi (paragi@sol.cc.u-szeged.hu)

Course description: The primary goal of the course is to provide an overview for doctoral students about *i)* the precise theoretical background of density functional theory; *ii)* the limitations of its applications; *iii)* some current theoretical research directions. As a result, students will be able to critically apply the Density Functional Theory during electronic structure problems.

Topics:

1. Brief introduction to functionals: Mathematical background; functional derivative; role of functionals in physics.
2. Schrodinger equation for atoms and molecules: Reduction of the number of variables. Stationary case, adiabatic and Born-Oppenheimer approximation, independent particle model.
3. Theoretical background of the Hartree-Fock method, the terms of the Fock operator.
4. Derivation of the Hohenberg−Kohn theorems for non-degenerate, ground state N-electron systems.
5. The early stage of Density Functional Theory: Derivation of the Thomas−Fermi kinetic functional.
6. The Kohn−Sham picture. Derivation of the Kohn−Sham equations.
7. Exchange functionals in Density Functional Theory: The local density approximation. Derivation of the Xα energy functional.
8. Beyond the local density approximation: Functionals with gradient corrections. Hybrid functionals.
9. Correlation in Density Functional Theory.: Local Density Approximation and Gradient corrections.
10. Investigation of excited state systems: ensemble Density Functional Theory; The fundamentals of linear response theory.
11. Outlook on some current research directions: Density matrix functional theory. Strongly Interacting Electron systems and its Kohn−Sham picture.

Literature:

- Robert G. Parr, Weitao Yang: Density-Functional Theory of Atoms and Molecules (Oxford University Press, 1989)
- Reiner M. Dreizler, Eberhard K. U. Gross: Density Functional Theory: An Approach to the Quantum Many-body Problem
  (Springer Berlin, Heidelberg,1990)

- Carsten Ullrich: Time-dependent density-functional theory: Concepts and Applications
  (Oxford University Press, 2012)