Density Functional Theory

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In this course I will explain the theoretical aspects of Density Functional Theory (DFT). The foundations of DFT will be built up from general considerations, to help you understand how DFT fits in a larger picture of methods aiming to deal with the quantum many-particle problem. We will go through the derivation of the Kohn-Sham equations and discuss their function and importance for the performance of practical DFT. I will also explain the philosophy used in the construction of basic approximations to the remaining exchange-correlation functional (LDA, GGA, hybrid) and point out important features of their performance. If time permits, I will also discuss the interpretation of the Kohn-Sham orbitals and orbital energies.

Prerequisites for attending the lecture: Basic Quantum Mechanics, basic linear algebra and Lagrange multipliers (Wikipedia / lectures notes Appendix B)