ISC 5935: Introduction to Density Functional Theory

What is Density Functional Theory?

The course is designed for materials scientists, chemists, physicists, and applied mathematicians who are seeking to know both the basic concept and certain advanced topics in density functional theory. Density functional theory (DFT) is widely used nowadays in both industry and academia to simulate various properties of materials and molecules, such as electronic properties, crystal structures, and chemical reactions.

Purpose of the Course

- We will learn the foundation of DFT. We will discuss several key concepts in DFT, including band gap, fractional electron number, and self-interaction error.
- The numerical aspects of DFT will be discussed in detail. We will learn two popular of basis sets, i.e., Gaussian basis and plane-wave basis, for performing DFT.
- We will learn how to perform DFT calcualtions on small molecules and simple solids. We will learn how to calculate basic properties of solids and free energies of molecules.
- Several frontiers in DFT will be covered, including orbital-dependent exchange-correlation functionals and orbital-free density functional theory.

List of Topics:

1. Basic concepts in DFT: Hohenberg-Kohn theorem, Levy-Lieb constrained-search formulation of DFT, Kohn-Sham equation, and spin-polarized DFT.
2. Exchange correlation functionals: local density approximation (LDA), hybrid exchange correlation functional, self-interaction correction, LDA+U, and van der Waals functionals.
3. Orbital-dependent exchange correlation functionals: optimized effective potential problem, exact exchange, and random phase approximation.
4. Basics of solids state physics, Bravais lattice, reciprocal space, Bloch theorem, and Brillouin Zone.
5. Pseudopotentias: norm-conserving pseudopotential, nonlinear core correction, and project-augmented wave technique.
6. Numerical aspects of Kohn-Sham DFT: smearing, *k*-point sampling, Gaussian basis set, and plane-wave basis set.
7. Geometry optimization in DFT: Hellmann-Feynman force, Pulay force, and stress.
8. Orbital-free density functional theory.
9. *Ab initio* molecular dynamics, Car–Parrinello molecular dynamics.
10. Potential-functional formalism of DFT and the physical meaning of Kohn-Sham eigenvalues.
11. DFT for fractional number of electrons.
12. Application of DFT: vibrational frequencies, enthalpy, and Gibbs free energy of molecules. Bulk modulus, shear modulus, phase transition pressure, reaction barrier, vacancy formation energy, surface adsorption energy, and surface energies.

Reference:

- "Density-Functional Theory of Atoms and Molecules" by Parr and Yang.
- "The ABC of DFT", by Kieron Burke, http://dft.uci.edu/doc/g1.pdf
- "Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory", Szabo and Ostlund.

Supplementary References:

- "A bird's-eye view of density-functional theory" by K Capelle, Brazilian Journal of Physics 36, pp 1318 (2006).
- "Challenges for Density Functional Theory", Cohen et al., Chemical Review 112, pp 289 (2012).
- "Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients", Payne et al., Review of Modern Physics 64, pp 1045 (1992).
- "Random-phase approximation and its applications in computational chemistry and materials science", Ren et al., Journal of Materials Science 47, pp 7447 (2012).
- "Orbital-dependent density functionals: theory and applications" Kümmel and Kronik, Review of Modern Physics, 80, pp 3 (2008)

Grading:

- Homework: 10 homework assignments (50%)
- Mid-term written exam (25%)
- Final project (25%)

Instructor:

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