ISC 5473
Introduction to Density Functional Theory
Spring 2021

SYLLABUS

Instructor   Chen Huang
              484, Dirac Science Library
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Class   Tuesday (face-to-face) and Thursday (Zoom-based): 1:20-2:35 pm
              (Zoom links have been created on Canvas)

Office Hours   1) Thursday 2:45-3:45 pm (Zoom links have been created on Canvas)
              2) or simply set up a time with Chen Huang by email.

Website   FSU Canvas Course Management Site.

Objectives

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. In this course, you will learn both the theoretical and numerical aspects of DFT. We will also learn how to perform DFT calculations on simple molecules and solids using DFT programs such as NWChem and ABINIT.

Topics to be discussed

The first class is on 1/7 (Thursday) and the last class is on 4/15 (Thursday). Here is a tentative list of topics to be covered.

- Basic concepts in DFT: Hohenberg-Kohn theorem, Levy-Lieb constrained-search formulation of DFT, Kohn-Sham equation, and spin-polarized DFT.

- Exchange correlation functionals: local density approximation, hybrid exchange-correlation functional, self-interaction correction, etc.

- Orbital-dependent exchange correlation functionals: optimized effective potential, exact exchange, and random phase approximation.

- Basics of solids state physics: Bravais lattice, reciprocal space, Bloch theorem, and Brillouin zone.

- Pseudopotentias: norm-conserving pseudopotential, nonlinear core correction, and project-augmented wave technique.

- Numerical aspects of Kohn-Sham DFT: smearing, k-point sampling, Gaussian basis set, and plane-wave basis set.

- Geometry optimization: Hellmann-Feynman force, Pulay force, and stress.

- *Ab initio* molecular dynamics.

- Physical meaning of Kohn-Sham eigenvalues, and fractional number of electrons.

- Applications: vibrational frequencies, enthalpy, and Gibbs free energy of molecules. Bulk modulus, shear modulus, phase transition pressure, reaction barrier, vacancy formation energy, surface adsorption energy, surface energies, and charge analysis.

References

- "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`

Supplementary References

- "Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory", Szabo and Ostlund.

- "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).

- "Orbital-dependent density functionals: theory and applications" Kümmel and Kronik, Review of Modern Physics, 80, pp 3 (2008)

- "Random-phase approximation and its applications in computational chemistry and materials science", Ren et al., Journal of Materials Science 47, pp 7447 (2012).

Grading Policy

- Homework 60%

- Midterm 20%

- Final project 20%

A: More than 90% overall, B: 80% to 89%, C: 70% to 79%, D: 60% to 69%, F: less than 60%. If you think you haven't received the credit you deserve for a homework or an exam, write up your argument, and submit for re-grading no later than 3 days after the graded assignments have been handed out.

Late Assignment Policy

No assignments will be accepted more than 7 days past the due date. Exceptions to these rules are made only if extenuating circumstances (such as illness, etc.) arise which can be documented. For a late assignment, it will be penalized by applying a graded scale which terminates with a 25% reduction at the end of one week.

University Attendance Policy

Excused absences include documented illness, deaths in the family and other documented crises, call to active military duty or jury duty, religious holy days, and official University activities. These absences will be accommodated in a way that does not arbitrarily penalize students who have a valid excuse. Consideration will also be given to students whose dependent children experience serious illness.

Academic Honor Policy

The Florida State University Academic Honor Policy outlines the University's expectations for the integrity of students' academic work, the procedures for resolving alleged violations of those expectations, and the rights and responsibilities of students and faculty members throughout the process. Students are responsible for reading the Academic Honor Policy and for living up to their pledge to ". . . be honest and truthful and . . . [to] strive for personal and institutional integrity at Florida State University." (Florida State University Academic Honor Policy, found at `http://dof.fsu.edu/honorpolicy.htm`.)

Americans With Disabilities Act

Students with disabilities needing academic accommodation should:

- register with and provide documentation to the Student Disability Resource Center; and

- bring a letter to the instructor indicating the need for accommodation and what type. This should be done during the first week of class.

This syllabus and other class materials are available in alternative format upon request. For more information about services available to FSU students with disabilities, contact the:

> Student Disability Resource Center
> 874 Traditions Way
> 108 Student Services Building
> Florida State University
> Tallahassee, FL 32306-4167
> (850) 644-9566 (voice)
> (850) 644-8504 (TDD)
> sdrcadmin.fsu.edu
> `http://www.disabilitycenter.fsu.edu`

Free Tutoring from FSU For tutoring and writing help in any course at Florida State University, visit the Academic Center for Excellence (ACE) Tutoring Services' comprehensive list of tutoring options - see `http://ace.fsu.edu/tutoring` or contact `tutor@fsu.edu` for more information. High-quality tutoring is available by appointment and on a walk-in basis. These services are offered by tutors trained to encourage the highest level of individual academic success while upholding personal academic integrity.

Syllabus Change Policy

Except for changes that substantially affect implementation of the evaluation (grading) statement, this syllabus is a guide for the course and is subject to change with advance notice.