Fall 2021

CHEM 567/PHYS 581/NSMS 595

Advanced Topics: Density Functional Theory

Tues./Thurs. 4:00-5:15 PM; in person and virtual; location TBA

Instructor: Prof. Susan R. Atlas, Department of Chemistry & Chemical Biology and Department of Physics & Astronomy

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Course Description

This 3-credit course is aimed at students and researchers interested in learning about the theory and application of density functional theory (DFT) for performing large-scale electronic structure calculations and structural studies of molecular and condensed phase systems. The foundational theorems of DFT established the existence of (1) a universal exchange-correlation functional encoding the full quantum complexity of the many-electron wavefunction; and (2) a mapping of the electronic structure problem onto a set of Hartree-Fock-like single-particle equations, the Kohn-Sham (KS) equations. DFT's development and implementation were recognized with the Nobel Prize in 1998, and the methodology is now the *de facto* standard for performing quantum mechanical calculations in complex atomic environments. Examples of properties that can be studied using DFT include charge polarization, charge transfer, excited states, and charge transport; the electronic structure of quantum dots and other mesoscale structures; band gaps in semiconductors; ligand-protein binding for rational drug design; and the interplay of spin, charge, and structure in alloys, grain boundaries, and high-T_c superconductors. Calculations can be performed using DFT alone, or by coupling DFT to classical molecular dynamics (MD) simulations.

The course will be organized as an advanced seminar, with 30 regular lectures, 3 supplementary computational lectures, and 5 workshop/labs. The majority of the course grade will be based on a theoretical/computational term project (term paper + oral presentation during finals week) determined by the student's research interests.

I. *Fundamentals* [18 lectures]. Atomic, molecular, and condensed matter electronic structure problems. Hartree-Fock theory. Hohenberg-Kohn and Kohn-Sham theorems. Excited states and time-dependent DFT (TDDFT).

II. *Functionals* [12 lectures]. Functional design criteria and strategies. Model-based functionals. Hybrid functionals. Selecting functionals for specific applications.

III. *Computation* [3 supplementary lectures; 5 workshop/labs]. Labs will be held outside regular lecture hours, and will utilize the supercomputing resources of the UNM Center for Advanced Research Computing (CARC). The instructor will be available for consultation and assistance. An "Intro to CARC" presentation will be included in the workshop/lab series. This course component will prepare students for independent work on their computational term projects. Codes introduced in the course will include `abinit`, `Gaussian`, and `Octopus`.

Prerequisites: One semester of quantum mechanics at the level of undergraduate physical chemistry or beyond (strongly recommended); experience with a high-level programming language (e.g., C, C++, Fortran 90; Matlab) and scripting (e.g., `perl`, `Python`, `tcsh`) helpful but not required. Please email the instructor with any questions about the course.