Fall 2025

CHEM 567/PHYS 581/NSME 595

Advanced Topics: Density Functional Theory

Tues./Thurs. 5-6:15 PM; PAÍS 1160

Instructor: Prof. Susan R. Atlas, Department of Chemistry & Chemical Biology, Department of Physics & Astronomy, and Center for Quantum Information & Control

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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. DFT is the *de facto* standard for studying the quantum mechanical ground and excited state behavior of intereacting electron systems, and rests on formal theorems establishing 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, which are the equations solved in practice. The ground state theory was subsequently extended to excited states. DFT's development and implementation were recognized with the Nobel Prize in 1998.

The course will be organized as an advanced seminar, with 25 regular 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* [15 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* [10 lectures]. Functional design criteria and strategies. Model-based functionals. Hybrid functionals. Selecting functionals for specific applications.

III. *Computation* [5 workshop/labs]. Labs will utilize the supercomputing resources of the UNM Center for Advanced Research Computing (CARC). 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 `pySCF/libxc`.

Prerequisites: One semester of quantum mechanics at the level of undergraduate physical chemistry or beyond. 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.