Fundamentals of Density Functional Theory and Green's Function Formalism

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Course Objective:
The course is an introduction to Density Functional Theory (DFT) and Green's function technique, both are essential for describing the electronic structure of real materials from first principles. The former is the method of choice for computing ground-state properties while the latter is suitable for describing spectroscopic properties. A wide range of materials properties can nowadays be computed using these two approaches.

Learning Goals:
At the end of the course, the students are expected to:
1. understand key concepts in Density Functional Theory and Green's function formalism.
2. be familiar with theoretical schemes for computing the electronic structure of real materials from first principles.
3. be able to comprehend literature on electronic structure and have the knowledge for applying the learned schemes to real problems.

Class Plan:
Day 1: Introduction; Review of occupation number representation, functional derivative
Day 2: Mean-field methods: Hartree and Hartree-Fock approximations.
Day 3: DFT 1: Hohenberg-Kohn theorem, Kohn-Sham scheme
Day 4: DFT 2: Formal expression for exchange-correlation energy, exchange-correlation hole, local density approximation
Day 5: Green's function 1: Basic definitions, equation of motion, functional derivative technique.
Day 6: Green's function 2: Linear response theory, Kubo formula, random-phase approximation
Day 7: Green's function 3: *GW* approximation, lecture on the *GW* method.

Literature:
-Compendium for the course will be provided
-R. M. Martin: "Electronic Structure: Basic Theory and Practical Methods" (Cambridge)

Grading Policy:
40%: class participation; 60 % home assignments