short course on density-functional theory

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Lecture 1: *Mathematical preliminaries*

- functionals and functional derivatives
- variational principles and the (generalized) Hellmann-Feynman theorem
- constrained minimization and Lagrange multipliers
- Legendre transforms

Lecture 2: *Density-functional theory*

- the electronic ground state as a functional of the external potential
- the Hohenberg-Kohn density functional
- the Kohn-Sham ansatz and equations and the exchange-correlation energy functional
- pair correlations, correlations holes, and energy functionals

Lecture 3: *Density-functional perturbation theory*

- derivatives of the total energy from the Hellmann-Feynman theorem
- higher-order derivatives from (density-functional) perturbation theory
- the 2n+1 theorem
- lattice dynamics from DFPT
- polar materials and the effect of macroscopic electric fields

Lecture 4: *Time-dependent density-functional (perturbation) theory*

- excited states and spectroscopy
- the Runge-Gross theorem
- perturbation theory: TD-DFT vs. RPA
- the quantum Liouville equation
- Casida's equations
- the Liouville-Lanczos approach to TD-DFPT

Lecture 5: *Dispersion forces and Van der Waals interactions*

- dispersion forces in quantum and classical physics
- the quantum fluctuation-dissipation theorem
- the adiabatic-connection fluctuation-dissipation (ACFD) approach to DFT
- the ACFD-DFT approach to dispersion forces
- non-local Van der Waals energy functionals