

Department of Chemical Sciences

Graduate course, Spring 2020

METHODS OF ELECTRONIC STRUCTURE THEORY

Central Topics:

- Many-body problem and electron correlation
- Concept of potential energy surface
- Theories of chemical bonding
- Mean-field and semi-empirical methods
- Approximate wavefunction methods for electron correlation
- Introductory density functional theory
- Molecular properties
- Intermolecular interactions

Suggested Text Books:

1. Attila Szabo and Neil S. Ostlund, *Modern Quantum Chemistry*, Dover, 1996.
2. Ira N. Levine, *Quantum Chemistry*, Pearson, 7th ed., 2016.
3. Frank Jensen, *Introduction to Computational Chemistry*, Wiley, 3rd ed., 2007.
4. Roy McWeeny, *Methods of molecular quantum mechanics*, Academic Press, 2nd ed., 1992.
5. Trygve Helgaker, Paul Jørgensen, and Jeppe Olsen, *Molecular electronic-structure theory*, Wiley, 2000.
6. Anthony J. Stone, *Theory of Intermolecular Forces*, Oxford University Press, 2nd ed., 2013.
7. Eberhard Engel, Reiner M. Dreizler, *Density Functional Theory: An Advanced Course*, Springer Berlin Heidelberg, 2011.

Prerequisites: Linear algebra and basic quantum chemistry.

Grading Policy: Assignments (30%), Midterm (35%), Final (35%).

Venue: AG80

Hours: Mon, Thu 11:30 am – 1:00 pm,

Office Hours: Tue, Fri (2–3 pm) or set up an appointment via email

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First lecture on Jan 20th (Monday)