Department of Chemical Sciences

Graduate course, Spring 2019

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 ab initio 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. Frank Jensen, *Introduction to Computational Chemistry*, Wiley, 3rd ed., 2007.
3. Roy McWeeny, *Methods of molecular quantum mechanics*, Academic Press, 2nd ed., 1992.
4. Trygve Helgaker, Paul Jørgensen, and Jeppe Olsen, *Molecular electronic-structure theory*, Wiley, 2000.
5. Anthony J. Stone, *Theory of Intermolecular Forces*, Oxford University Press, 2nd ed., 2013.
6. 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 (30%), Final (40%).

Venue: AG80
Hours: Tue 10:00 am – 11:15 am,
Thu 11:15 am – 12:30 pm
Office Hours: Wed, Fri (2–3 pm) or set up an appointment via email

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The first lecture starts on Jan 22nd (Tuesday)