Department of Chemical Sciences

Graduate course, Spring 2022

METHODS OF ELECTRONIC STRUCTURE THEORY

vkvoora.github.io/teaching/mest/

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
- Modern computational tools for quantum chemistry

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: AG66 or online
Time: Tue, Fri 11:30 am – 1:00 pm
Office Hours: Tue, Fri (2–3 pm) or set up an appointment via email

Instructor: Vamsee Voora (vamsee.voora@tifr.res.in, Office NMR201, extn: 2978)
TA: Ritaj Tyagi (ritaj.tyagi@tifr.res.in; Office D225)

First lecture on Jan 18th (Tuesday)