

CHM 627A

Methods Of Electronic Structure Calculation

First course handout

Instructor: Mainak Sadhukhan

Indian Institute of Technology Kanpur

- Recapitulation of Linear algebra and quantum mechanics of Hydrogenic atoms
- Hartree-Fock Theory of many-electron systems
- Electron correlation and some beyond-Hartree-Fock theories
- Electron density-based methods
- An in-house code will be written to calculate energy of a simple system, if time permits.

- Assignments may be given for practice
- Two project presentation will be conducted, each containing 25% marks
- No mid-sem examination will be arranged
- End-semester examination will cover 50% marks
- No pro-rating is admissible
- End-sem make-up can only be admissible for medical emergency, properly approved by authorities (SPGC/SUGC)

Books

- ① Modern Quantum Chemistry, A. Szabo and N. L. Ostlund, Dover, New York (1996).
- ② Density Functional Theory of Atoms and Molecules, R. G. Parr and W. Yang, Oxford University Press, Oxford (1986).
- ③ Molecular Electronic Structure Theory, T. Helgaker, J. Olsen and P. Jorgensen, Wiley, New York (2013).

Online resources

The instructor will mention possible online resources during teaching.

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The students are very much encouraged to contact the instructor whenever needed