Chemical Binding (CY524)

Instructor: P. Manikandan Office: 3103, Admin. Block. ☎ 282 ✉ pmanikandan@iitj.ac.in

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✓ Contents

- ⊛ Many electron atoms, Variational principle, Born-Oppenheimer approximation, H_2^+ ion, homo and hetero nuclear diatomic molecules, Valence bond and Molecular orbital theories
- ⊛ Hartree-Fock (HF) theory of atoms and molecules, Self-consistent field (SCF) wavefunction, configuration interaction (CI) wavefunction, Moller-Plesset perturbation theory and CI calculations
- ⊛ Introduction to Semi-empirical methods, CNDO (Complete neglect of differential overlap), INDO (Intermediate neglect of differential overlap) and NDDO (Neglect of of diatomic differential overlap) methods
- ⊛ Principles of density functional theory (DFT), Commercial functionals
- ⊛ Time dependent perturbation theory, Transition probability and Reaction cross section
- ⊛ Intermolecular forces and their determination
- ⊛ Use of Gaussian and other public domain software to perform simple electronic structure calculations

✓ Grading

Midsem I	20 points
Midsem II	20 points
Endsem	50 points
Assignments	10 points
Total	100 points

✓ Books

- ⊛ I. N. Levine, *Quantum Chemistry*, Pearson education (2006).
- ⊛ J. P. Lowe and K. A. Peterson, *Quantum Chemistry*, Academic Press (2005).
- ⊛ A. Szabo, and N. S. Ostlund, *Modern Quantum Chemistry*, Dover (1996).

Note: In addition to the above books, relevant research articles will be provided occasionally.

The underlying physical laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations that are much too complicated to solve. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed...

— *P. A. M. Dirac* (1929)