



Department of Chemical Sciences

2019 Graduate Course in

QUANTUM CHEMISTRY-1



J. Neaton and L. Venkatraman
Nano Lett. 2014

Gregory Engel,
University of Chicago

Course Description

The course will emphasize the importance of learning quantum mechanics for chemists. Modern experiments will be used as a motivation to discuss the conceptual basis of quantum explanations and provide tour of the language associated with it.

Topics to be covered

- Need for a quantum theory in view of modern experiments, Discreteness in classical systems
- Dynamics of classical particles, tracking classical trajectories, electron motion, Formulation of the Quantum theory; Defining Operators
- Quantum Mechanics of Simple Systems, Harmonic Oscillator
- Angular Momentum, Spherical Harmonics
- Theory of One Electron Systems
- Variation and Perturbation Method; Transitions and Fermi-Golden rule
- Diatomic Molecules, symmetry and associated quantum chemistry of many electron systems
- Hartree-Fock Methods
- Semi-empirical M.O. Calculations

Suggested Text Books:

'Elementary Quantum Chemistry', Frank Pilar, McGraw-Hill, 1990

'Quantum Chemistry', Ira Levine, Prentice Hall India, 2008

'Molecular Quantum Mechanics', by PW Atkins and R. Friedman, Oxford University Press, 2007

'Quantum Chemistry' by A.B. Sannigrahi, Books and Allied, 2010

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Tutors: Mr. Pulkit Joshi and Ms. Sunandita Paul

Venue: Lecture room AG80; First class 7th August 2019

Days: Wednesdays and Fridays;

Time: Wed 11:30 am to 1 pm and Fri 9:30 am to 11:00 am

Tutorials: Monday 9:30 am to 11 am