



J. Neaton and L. Venkatraman
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Department of Chemical Sciences

2017 Graduate Course in

QUANTUM CHEMISTRY



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

- New experiments and need for understanding quantum chemistry, review of classical mechanics and formulation of the theory
- Operators; Theorems of Quantum Mechanics
- Quantum Mechanics of Simple Systems, Harmonic Oscillator
- Angular Momentum, Spherical Harmonics
- Theory of One Electron Systems
- Variation and Perturbation Method
- Diatomic Molecules and associated quantum chemistry of many electron systems, potential energy surfaces
- 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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Venue: Lecture room AG80

Days: Wednesdays and Fridays

Time: 11:00 hr to 12:30 hr

First lecture starts on 9th August 2017.