Quantum Chemistry and Spectroscopy (CY514)

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✓ Contents

- ⊛ Old quantum theory, Correspondence principle, Bohr-Sommerfeld quantization, Wave-particle duality, and Stern-Gerlach experiment
- ⊛ Operators, Eigenfunctions and eigenvalues, Operators in quantum mechanics, and Expectation values
- ⊛ Time independent and time dependent Schrödinger equation, Particle confined to infinite and finite potential wells, Harmonic oscillator, Rigid rotor, and Hydrogen atom
- ⊛ Variational principle, Perturbation theory, Energy and wavefunction corrections
- ⊛ Born-Oppenheimer approximation, Hartree-Fock self-consistent field method, Electron correlation, Spin-orbit interaction, and Density functional theory
- ⊛ Introduction to rotational, vibrational, and NMR spectroscopy, Electronic transitions, Frank-Condon principle, Vertical transitions, Selection rules, Parity, Symmetry and spin selection rules, Jablonski diagram, and Beer-Lambert law

✓ Grading

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

- ⊛ Present your assignments clearly and they have to be detailed enough. Assignment submission dates are non-negotiable.
- ⊛ Assignment problems are NOT an exhaustive list of problems. One should be doing more problems in addition to the assignments. Refer standard books.

✓ Text Book

- ⊛ *Quantum Chemistry*, I. N. Levine, Pearson Education India, 7^{th} Edition (2016).

✓ Reference Books

- ⊛ *Principles of Quantum Mechanics*, R. Shankar, Springer, 2^{nd} edition (1994).
- ⊛ *Quantum Chemistry*, D. A. McQuarrie, Viva Books, 2^{nd} edition (2016).
- ⊛ *Quantum Mechanics*, A. Messiah, Dover Publications Inc. (2014).
- ⊛ *Modern Quantum Mechanics*, J. J. Sakurai and J. J. Napolitano, Pearson Education India, 2^{nd} edition (2013).
- ⊛ *Spectra of Atoms and Molecules*, P. F. Bernath, Oxford University Press USA, 3^{rd} edition (2016).

✓ Fun Reading ☺

- ⊛ *Alice in Quantumland*, R. Gilmore, Copernicus, (1995).

- ⊛ *In Search of Schrödinger's Cat*, J. Gribbin, RHUK, Updated edition (1985).
- ⊛ *Schrödinger's Kittens and the Search for Reality*, J. Gribbin, Orion Publishing Group (2003).
- ⊛ *Mr Tompkins in Paperback*, G. Gamow, Cambridge University Press, Reprint edition (2012).

I think I can safely say that nobody understands quantum mechanics

— Richard Feynman