Department of Chemistry Indian Institute of Technology Kanpur Session 2017-2018, Semester – I

CHM 321A/421A Physical Chemistry – I

Lectures: MWF 10:00 - 11:00 am L14

Instructor: Dr. Pratik Sen Office: OldCoreLab 101B Tel: 6312 Email: psen@iitk.ac.in

Course Details:

- Introduction: importance, historic background, quantum mechanics vs classical mechanics, wave particle duality, uncertainty principle
- Schrödinger equation: wave function and interpretation, time dependent and time independent Schrödinger equation, eigen value problem
- Quantum mechanics of some simple systems: free particle, particle in a box, harmonic oscillator
- Angular Momentum: rigid rotor, orbital and spin angular momentum
- Hydrogen and hydrogen like atoms
- Approximate methods: perturbation theory, variation method, some simple examples.
- Many electron atom: Pauli anti symmetry principle, Slater determinant, He atom. Li atom.

Text Book:

• N. Levine, Quantum Chemistry

Grading System:

• Quiz: 10% + 10%

MSE: 30%ESE: 50%

Letter Grade:

• Awarded based on the total marks out of 100.