QUANTUM CHEMISTRY OF ATOMS AND MOLECULES

INTENDED AUDIENCE: Chemistry, Physics, 1st year Engineering

COURSE OUTLINE:
The course introduces students to quantum Chemistry. The syllabus is as follows.
Black body radiation. Failure of classical mechanics. Marsden experiment and Rutherford theory.
Schrodinger equation. Postulates of quantum mechanics. Born approximation. Origin of quantization:
Molecular orbitals of homonuclear and heteronuclear diatomic molecules. VSEPR. Molecular orbital and
Valence bond approaches to polyatomic molecules. Hybrid orbitals. Huckel theory. Introduction to
approximation methods. Scope of further study.

ABOUT INSTRUCTOR:
Prof. Anindya Datta is a Professor of Chemistry in IIT Bombay, with research interest in ultrafast
spectroscopy and time resolved fluorescence microscopy. I have teaching experience of 17 years. 14 Ph.
D. students have graduated from our laboratory. Eight more are working towards their degree. I received
Excellence in Teaching Award from our institute in 2017 and have taught two NPTEL courses: one on
Molecular Spectroscopy and another on Symmetry in Chemistry.

COURSE PLAN:

Week 1: Black body radiation. Failure of classical mechanics. Marsden experiment and Rutherford theory.
Week 3: Schrodinger equation. Born approximation.
Week 4: Postulates of quantum mechanics. Introduction to operator algebra.
Week 5: Origin of quantization: Particle in a box, particle in a ring.
Week 6: Hydrogen atom.
Week 8: Introduction to spin. Slater determinants. Self consistent fields.
Week 9: Valence bond and molecular orbital theories. Molecular orbitals of homonuclear and
heteronuclear diatomic molecules.
Week 10: VSEPR. Molecular orbital and Valence bond approaches to polyatomic molecules. Hybrid
orbitals.
Week 11: Huckel theory.
Week 12: Introduction to approximation methods. Scope of further study.