

Course Title	Quantum Chemistry			Course No.				
Center	Chemistry Focus group			Structure	3	0	0	4
Offered for	PhD			Status	Core		<i>Elective</i> ✓	
Faculty Member Offering	Chemistry Focus group			Type	<i>New</i>		Modification ✓	
Pre-requisite	<i>Vectors, Linear algebra</i>			To take effect from				
Submitted on	Focus Group Approval on	Center Approval on	AC approval on	Senate approval on				

Objectives

1. The course is an attempt to provide an advanced level understanding of quantum chemistry.
2. Emphasis will be on applications of quantum mechanics to chemistry and solid state physics.

Learning Outcomes

Understanding of quantum mechanics and applications to chemistry problems such as energy and geometry optimizations.

Course Content:

Fundamentals of Quantum Mechanics: Failure of classical physics - Postulates of Quantum Mechanics – Measurement Process.

Exactly solvable problems – Approximation methods

Many electron atoms – Hartree-Fock-Roothan equations and basis sets – Huckel Theory

Electronic structure theory – *Ab Initio* methods – Moller-Plesset perturbation theory – Density Functional theory – Path Integrals

(A few lab sessions will be planned depending on the availability of resources and time)

Reference Books

1. P. W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press, 1983.
2. I. N. Levine, *Quantum Chemistry*, Allyn and Bacon, 1983.
3. D. A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983.
4. G. Schatz, *Quantum Mechanics in Chemistry*, Dover Books, 2002.