



# TIME DEPENDENT QUANTUM CHEMISTRY

## PROF. ATANU BHATTACHARYA

Department of Chemistry

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**PRE-REQUISITES** : Must have a fair idea of postulates of quantum mechanics (as given in Quantum Chemistry or Physical Chemistry book by McQuarrie).

**INTENDED AUDIENCE** : Physics/Chemistry UG PG students

**INDUSTRIES APPLICABLE TO** : Industries where quantum theory is extensively used.

### COURSE OUTLINE :

In our current course curriculum, except for time-dependent perturbation theory, physical chemistry students are not introduced to the time dependent quantum chemistry at all. This creates a big knowledge gap in students working on chemical dynamics, spectroscopy, and ultrafast spectroscopy fields. Objective of this course is to fulfil the knowledge gap not only by introducing the subject to them, but also by helping them use numerical methods to practically deal with some selected time-dependent quantum chemistry problems.

### ABOUT INSTRUCTOR :

Prof. Atanu Bhattacharya was born at Matiari (Nadia, West Bengal, India), in 1983. He received the BSc degree in Chemistry from R. K. Mission Vidyamandira (Calcutta University, India) and the MSc degree in Physical Chemistry from Indian Institute of Technology, Bombay (India), in 2003 and 2005, respectively. He received the PhD degree in Physical Chemistry from Colorado State University (USA) in 2010. His doctoral research involved the time and frequency resolved spectroscopy of energetic molecules in molecular beam under supervision of Prof. Elliot R. Bernstein. In 2010, he joined Department of Chemistry, Brookhaven National Laboratory (USA) as post-doctoral fellow for studying catalytic reaction dynamics in femtosecond to picosecond time domain under supervision of Dr. Nicholas Camillone III. Then in 2012 he joined Kyoto University (Japan) as program specific researcher to work on liquid beam time resolved photoelectron spectroscopy and liquid beam X-ray absorption spectroscopy under supervision of Prof. Toshinori Suzuki. In 2013, he joined Indian Institute of Science (Bangalore, India) as assistant professor at the Department of Inorganic and Physical Chemistry. Currently, he is an associate professor at the Department of Chemistry, GITAM University (Visakhapatnam, India). Dr. Atanu Bhattacharya, in his academic career, is specializing in Attosecond Chemistry, Femtosecond Chemistry of Catalysis and Explosives, Femtosecond X-ray Spectroscopy, Quantum Dynamics and Chemical Applications in Quantum Computer. He has taught the course "Time Dependent Quantum Mechanics" at the Indian Institute of Science for several years.

### COURSE PLAN :

**Week 1:** Introduction and the Time-Dependent Schrödinger Equation (Pure and Superposition States)

**Week 2:** Introduction to Quantum Dynamics with Classical Mechanical Flavor (Ehrenfest Theorem and Bohmian Mechanics), Python Tutorials

**Week 3:** Time-Dependent Quantum Mechanics of Translational Motion and Wave packet Dynamics for free particle, linear potential and harmonic potential, Python Tutorial on Fourier Transform

**Week 4:** Quantum Mechanics and Linear Algebra, Python Tutorial on Eigenvalue and Eigenfunction

**Week 5:** Numerical Solution to TDSE, Python Implementation of Wavepacket Dynamics

**Week 6:** Quantum Adiabatic Theory: Application with Particle in 1D Box.

**Week 7:** Electronically Nonadiabatic Transitions

**Week 8:** Electronically Nonadiabatic Transitions To Be Continued

**Week 9:** Time-Dependent Perturbation Theory: Light-Matter Interaction with Scalar and Vector Potential

**Week 10:** Light-Atom Interaction to be Continued

**Week 11:** Light-Atom Interaction to be Continued

**Week 12:** Time Correlation Function and Time Domain Approach to Spectroscopy