



TIME DEPENDENT QUANTUM CHEMISTRY

PROF. ATANU BHATTACHARYA

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IISc Bangalore

TYPE OF COURSE : New | Elective | PG

COURSE DURATION : 12 weeks (24 Jan' 22 - 15 Apr' 22)

EXAM DATE : April 24, 2022

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.

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 (HerrinFesta Theorem and Bohmian Mechanics)

Week 3: General Principles of Time-Dependent Quantum Chemistry (Time Evolution Operator, Heisenberg and Interaction pictures)

Week 4: Time-Dependent Quantum Mechanics of Translational Motion and Wave packet Dynamics for free particle, linear potential and harmonic potential

Week 5: Time-Dependent Perturbation Theory: Light-Matter Interaction with Scalar and Vector Potential

Week 6: Time Dependent Perspective of Quantum Theory of Scattering and Chemical Reactions

Week 7: Numerical Methods in Time Dependent Quantum Chemistry (Numerical Solution to TDSE)

Week 8: Reaction Rate Processes: Transition State Theory and Beyond

Week 9: Time Correlation Function and Density Matrix Formalism

Week 10: Nonadiabatic Dynamics (Landau-Zener Dynamics, Conical Intersections, AIMS Dynamics)

Week 11: Adiabatic Dynamics

Week 12: Quantum Dynamical Processes in Chemistry