APPROXIMATE METHODS IN QUANTUM CHEMISTRY

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TYPE OF COURSE : Rerun | Core | PG
COURSE DURATION : 8 Weeks (24 Jan' 22 - 18 Mar' 22)
EXAM DATE : 27 Mar 2022

PRE-REQUISITES : Introductory Quantum Chemistry

INTENDED AUDIENCE : MSc (Chemistry) students and Chemistry PhD students interested in theoretical and computational chemistry research

COURSE OUTLINE :

This course will introduce students to various approximate techniques in quantum chemistry. In particular, a thorough mathematical and physical foundation will be laid for variational principle, perturbation theory, and self-consistent field method. The strengths and weaknesses of the techniques will be discussed and each technique will be illustrated by examples from chemical bonding and molecular spectroscopy. Several applications of these methods will be discussed in the assignments.

ABOUT INSTRUCTOR :

Prof. Sabyashachi Mishra is currently working as an Associate Professor in the Department of Chemistry, IIT Kharagpur. He has obtained BSc (Chemistry Honours) from Ravenshaw college, MSc (Chemistry) from University of Hyderabad, and PhD (Theoretical Chemistry) from Technical University of Munich. He worked in University of Basel and Zurich as a Post-doctoral researcher. He has 8 years of experience in teaching quantum-chemistry and physical-chemistry based courses in IIT Kharagpur. His research interests include application of quantum chemistry in molecular physics, molecular spectroscopy, and biochemical processes.

COURSE PLAN :

Week 1**:** Review of quantum mechanics

Week 2**:** Variational principle

Week 3**:** Chemical bonding

Week 4**:** Perturbation theory

Week 5**:** Many electron systems

Week 6**:** Self-consistent field method

Week 7**:** Hartree-Fock-Roothan method

Week 8**:** Time-dependent perturbation theory