PMRF-ISSS Teaching Programme

Prime Minister Research Fellowship students' teaching requirement facilitated by the Institute of Smart Structures and Systems

Module PMRF-ISSS122/II/2024

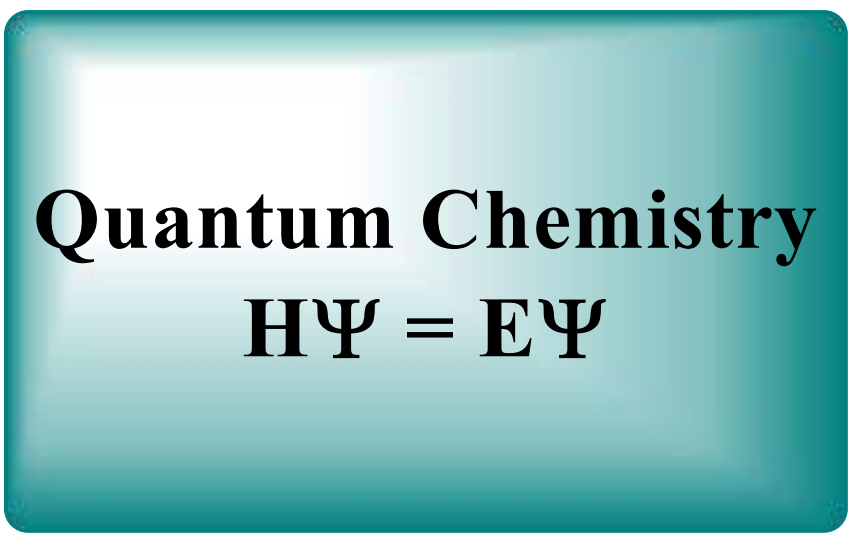
Quantum Chemistry

Name of the PMRF student

SAPNA

Required background of the students taught

B.Sc in Chemistry
M.Sc in Chemistry (not mandatory)



Details of the content of the module

Live lecture sessions on Quantum Chemistry:

Basic Quantum Chemistry: Basic postulates, eigenvalues and eigenvectors, Hermitian operators, applications including translational, vibrational and rotational degrees of freedom - particle in 1D/2D/3D box, particle in a ring, rigid rotor, harmonic oscillator. Solution of SchrÖdinger equation for the hydrogen atom; radial and angular functions, atomic orbitals and electron spin. Multi-electron systems.

Approximate techniques and chemical bonding: Born-Oppenheimer approximation, variation and perturbation methods with examples. Valence bond theory including mathematical treatment of sp, sp2 and sp3 hybridized orbitals, molecular orbital theory with suitable examples, uckel molecular orbital approach. Introduction to semi-empirical and ab initio methods.

Schedule of the module

Start date: 26th August 2024

End date(tentative): 23rd November 2024

Live lectures on Monday & Saturday: 9:00 AM – 10:00 AM

Meeting link : Will be shared later

Link

Contact email ID: isss.forum@gmail.com

sapna2022@iisc.ac.in

Registration link: https://forms.gle/bh4Hf7tjNa9Xv6M36