PMRF-ISSS Teaching Programme

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

Module PMRF-ISSS109/III/2025

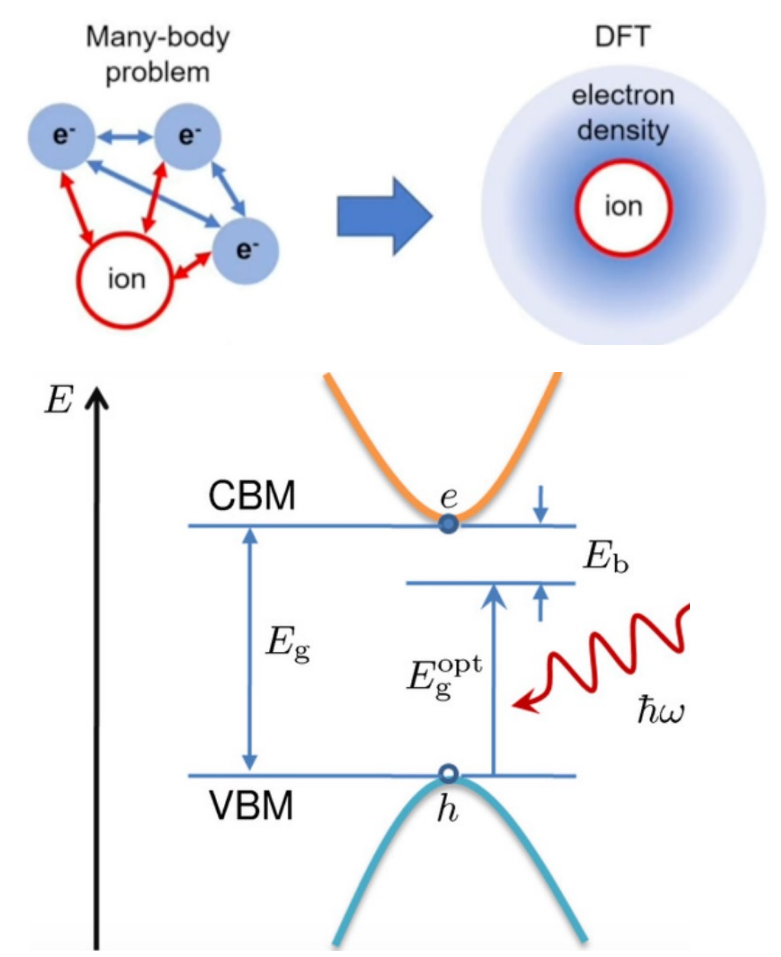
Density Functional and Many-Body perturbation theory

Name of the PMRF student

Robin Bajaj

Required background of the students taught

1. B.Sc. Physics (Honours)/ Major in Physics or Materials Science
2. B.Tech
3. Masters in Physics or/ Specialisation in Materials Science
4. Integrated PhD and PhD students with specialisation in Computational and theoretical condensed matter/ Materials Science



Details of the content of the module

1. Lectures 1-4: Intruduction to DFT, Hohenberg-Kohn theorems, Kohn-Sham equations, Exchange-correlation functionals, pseudopotentials, plane-waves
2. Lectures 5-6: DFT tutorials on QuantumEspresso, Practical calculations of Band structure, DOS etc.
3. Lecture 7: Symmetries in one-electron wavefunctions
4. Lecture 8-10: Introduction to MBPT, GW approximation, practical aspects
5. Lecture 11-12: GW tutorials in BerkeleyGW
6. Lecture 13-15: Bethe-salpeter equation, excitons, optical properties, absorption spectra
7. Lecture 16-18: Practical calculations/ Tutorials of GW-BSE
8. Lecture 19-20: Paper discussion on the Symmetries in excitons

Schedule of the module

Tentative schedule

Start date: 15 Nov 2025

End date: 18 January 2026

Lectures: Total 20 lectures every Saturday and Sunday (1-1.5 hour each depending on theory or tutorial)

Timings: 3:00-4:30 PM

Meeting link : Will be shared later

Contact email ID: robinbajaj@iisc.ac.in

Registration link: https://docs.google.com/forms/d/e/1FAIpQLScdUtPNE4eSGtX9g5QZPf0LGE8BdHykwnScVVfbjSP5zugwfA/viewform?usp=publish-editor