

Seminar

Topology, Optics and Magnetism in Quantum Materials from First principles

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Desiderata fuelling the search for novel two-dimensional topological materials have steered us to investigate the common facet that unifies the above compounds: existence of Dirac-like or Weyl-like points in the electronic spectrum and related topological properties. A detailed inspection of the fermiology, quantum oscillations and topological properties of the recently discovered Type II Weyl semimetals will be presented. Further, functional two-dimensional materials are promising for advanced atomically thin electronic and optoelectronic devices, such as light emitting diodes (LEDs), and valleytronic devices. We will discuss first-principles calculations based on density functional theory and many-body perturbation theory to investigate the optical properties and Auger recombination rates of layered materials by solution of the Dyson's equations. Finally, a thorough investigation of the energetics, magnetic moments and fully q -dependent spin susceptibility by the introduction of a novel methodology combining the random-phase approximation, and first principles calculations artificially stabilised by Hubbard interactions and spin-spiral calculations for the not yet foretold 2D Ising superconductor NbSe_2 will be narrated.

Friday, Dec 6th 2024

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Seminar Hall, TIFR-H