Topology and Optics in Two-Dimensional Oxides and Tellurides from First principles

Suvadip Das
George Mason University, Fairfax, USA

Abstract

Two-dimensional quantum materials such as MoS_2, WTe_2 and other transition metal dichalcogenides (TMDs) are reputed for atomically thin spintronic, valleytronic and quantum spin Hall devices. With the advent of quantum computing and superconducting devices, an exploration into the topological manifestation in 2D materials have been deemed indispensable. Desiderata fueling the search for novel two-dimensional topological materials have steered the investigation of popular layered Weyl semimetals $MoTe_2$ and WTe_2, and other new classes of layered materials. The common facet that unifies the above compounds is the fact that the low energy physics of these compounds is characterized by Dirac-like or Weyl-like points in the electronic spectrum and topological properties. This section of my presentation pertains to the study of the fermiology, quantum oscillations and topological properties of the recently discovered Type II Weyl semimetals $MoTe_2$ and WTe_2. Further, functional two-dimensional materials are promising for advanced atomically thin electronic and optoelectronic devices, such as light emitting diodes (LEDs), ultrathin solar cells, and valleytronic devices. Recently, atomic layers of α-PbO have been successfully grown for the first time using micromechanical and sonochemical exfoliation. We performed first-principles calculations based on density functional theory and many-body perturbation theory to investigate the electronic and optical properties (utilizing the GW and BSE methodology) of monolayer, bilayer, and bulk litharge α-PbO, including spin-orbit coupling effects. Strong excitonic binding energy was observed in monolayers of newly exfoliated α-PbO due to confinement. The α-PbO monolayer is nearly transparent in the visible and near UV, and absorbs strongly in the vacuum UV range, which is promising for solar-blind UV photodetectors. Finally, benchmarking studies of convergence of the quasiparticle self-consistent GW (QPscGW) method for prototypical bulk oxides MnO, CoO and NiO will be presented.