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Transport and scattering of confined electrons in electrides

Wednesday 29 May 2024 15:30 (30 minutes)

Electrides are unconventional ionic crystals with excess electrons that decouple from the atomic nuclei and fill voids in the lattice. With layered electrides, the excess electrons form 2D delocalized sheets confined to the interstitial region between the atomic layers, or on their surfaces when exfoliated to form 2D electrides (known as "electrenes"). The spatial decoupling of the electrons from the lattice results in very low work function, high conductivity, and weak electron-phonon coupling. High throughput screening has expanded the number of known electrides from a few to a few hundred and has identified electrides that are magnetic, semiconducting, topologically nontrivial, and superconducting. As a result, electrides are promising material candidates for applications related to transparent conductors, solid-state dopants, 2D semiconductor contacts, electron emitters, and interconnects. In this talk, I will present our recent efforts exploring the unusual transport and electron-phonon scattering characteristics of layered electrides using density functional theory.

Keyword-1

Density functional theory

Keyword-2

Transport

Keyword-3

Scattering

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