Hessisches Kompetenzzentrum
für Hochleistungsrechnen

High-Throughput Discovery of Mab and Mbene Superconductors

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Project Term
2022 - 2023

Clusters
Lichtenberg II Cluster Darmstadt

Software
VASP, Quantum ESPRESSO, ALAMODE

Additional Software
EPW

Institute
Theory of Magnetic Materials

University
Technische Universität Darmstadt, University of South Carolina

Introduction

We survey the landscape of MAB and Mbene superconductors out of our previous high-throughput predictions using first-principles calculations. To discover the superconducting behavior of MAB and Mbene phases, we performed DFT calculations to evaluate the electron-phonon interaction and to solve the anisotropic Migdal-Eliashberg equation to get the superconducting transition temperature. The current wort will shed light on the exploration of novel superconductors in borides.

Methods

The density functional theory (DFT) calculations were performed using the QUANTUM ESPRESSO (QE) and VASP packages. We adopted relativistic norm-conserving pseudopotentials with the PerdewBurke-Ernzerhof exchange-correlation functional in the generalized gradient approximation (GGA). The dynamical matrices for phonons and the linear variation of the self-consistent potential for electron-phonon coupling were calculated within the framework of density-functional perturbation theory (DFPT). The anisotropic Migdal-Eliashberg (ME) equation was solved to evaluate the superconducting properties with the EPW code. The most time-consuming parts of the project are the dynamic matrices setup and the electron-phonon interaction calculations, which scale cubic as the system size (i.e. number of atoms) grows.

Results

Before jumping into the superconductivity calculation of MAB and Mbene, we did a comprehensive study of the anharmonicity effect and electron-phonon interactions of some specific materials, which can help us generate the workflow and benchmark for next-step calculations. Among them, based on the electron-phonon Wannier interpolation and Boltzmann transport equation, the carrier mobilities and mode-resolved scattering rates of cubic $CsSnI_3$ and $CsPbI_3$ were calculated, and the dominant scattering channels were analyzed. Our results reveal that the mobility takes 595.9 and 84.5 cm^2/Vs at room temperature for $CsSnI_3$ and $CsPbI_3$, respectively, in good agreement with the experiment results. The longitudinal stretching mode of the Sn(Pb)-I bond with the frequency of 120 cm^{-1} plays a dominant role in carrier scattering. On the other hand, turning to two-dimensional material, we have systematically studied the electronic structures, phonon and charge transport properties, and thermoelectric properties of few-layered (from 1L to 4L) and bulk $PdSe_2$ by first-principles calculations and Boltzmann transport theory. As the thickness increases, the energy levels of band edges relative to 4s of selenium move oppositely due to their different bonding states, leading to the power-law decrease of the band gap. Meanwhile, the electron effective mass decreases rapidly while the hole effective mass increases significantly compared with those unperturbed. Calculations on elastic constants reveal that both bulk and few-layered $PdSe_2$ are mechanically stable, and the bulk is ductile with a Poisson's ratio of 0.27. The shifts of Raman active modes with respect to the thickness as well as their Gruneisen parameters, are analyzed, and the underlying physics is reported.

Discussion

From our studies, we understand that, compared with the harmonic approximation of atom interactions, the inclusion of strong anharmonicity leads to the enhancement of atom interactions, which decreases the EPC strength and consequently increases carrier mobilities. After understanding the anharmonicity effect and electron-phonon interactions, we are calculating the superconductivity properties of MAB and Mbene now. The manuscripts are being prepared and will be submitted soon.

Publications

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