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Thermoelectric Properties of Cd Based Zintl Phase Compounds

ABHISHEK SINGH, TRIBHUWAN PANDEY, Indian Institute of Science — Zintl phase compounds can be described as covalently-bonded anion substructures surrounded by highly electro-positive cations exhibiting essential features for thermoelectric applications. By combining first principles electronic structure and Boltzmann transport theory, here we report excellent thermoelectric properties of CdSb and ACd_2Sb_2 (where, A = Ca, Ba, Sr). The electronic structure shows heavy and light bands near the band edges, which lead to large power factor resulting in good thermoelectric performance. We also calculate lattice thermal conductivity by solving Boltzmann Transport equation using an iterative method. The large Grüneisen parameters and low phonon group velocity indicate strong anharmonicity in these compounds, which results in low lattice thermal conductivity. The low thermal conductivity and the excellent transport properties lead to a high ZT value of 1.9 in $CaCd_2Sb_2$ and $BaCd_2Sb_2$ at moderate p and n-type doping. These results indicate that well optimized Cd based Zintl phase compounds have a potential to match the performance of conventional thermoelectric materials.

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