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First-Principles Predictions of the Electronic, Optical and Thermoelectric Properties of the New Zintl-Phase Sr_2CdAs_2

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ABSTRACT

In this paper, we report results of a detailed first-principles study of physical parameters related to electronic and thermoelectric properties of the ternary distrontium cadmium diarsenide Sr_2CdAs_2. This compound crystallizes in the orthorhombic space group, *Cmc21* (No. 36, Z= 4). The equilibrium structural parameters are determined by CASTEP code, while the electronicstructure and related properties are investigated using Wien2k package. The energy band structure *Eg* = 1.44 eV with a direct bandgap. The thermoelectric parameters are investigated using thesemi-classical Boltzmann transport theory.

Introduction

Zintl phases compounds have a wide variety of interesting physical properties, such as photovoltaics and thermoelectricity, where the thermoelectric materials can be generating the electricity from the thermal energy (Heat) with high efficiency. Inthis paper, we report results of a detailed first-principles study of physical parameters related to electronic and thermoelectric properties of the ternary distrontium cadmium diarsenide Sr_2CdAs_2. This compound crystallizes in the orthorhombic space group, *Cmc21* (No. 36, Z= 4) 1.

Theoretical Study

The determined equilibrium structural parameters through thepseudopotential plane wave method within the density functional theory framework with the GGA-PBEsol functional are in excellent agreement with the available experimental counterparts, providing proof of the reliability of the reported results. The electronic structure and related properties are investigated using the full-potential linearized augmented plane wave plus localorbitals with the TB-mBJ potential. The microscopic origins of the electronic states involved in the direct interband optical transitions are identified. Dependencies of temperature and charge carrier concentrations of the thermoelectric parameters are investigated using the semi-classical Boltzmann transport theory.

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Results and DiscussionElectronic Properties

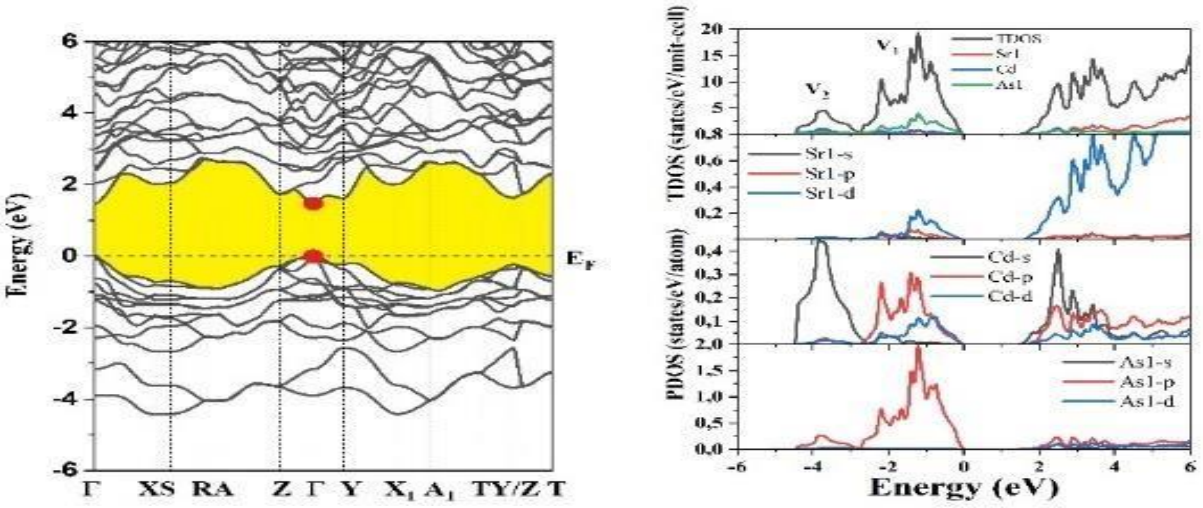

Fig. 1. Band structures calculated (left), the total density of states(TDOS) and its projections on orbitals and sites (PDOS) of Sr2CdAs2 (right) using the TB-mBJ potential. The Fermi level is set to zero.

Calculated energy band dispersions of Sr2CdAs2 the along a selected high symmetry path that connects points of high symmetry in the BZ is depicted in Fig. 1. Both VBM and CBMoccur at the BZ center; Γ-point, indicating that investigated compound is direct bandgap material *Eg* = 1.44 eV. The GGA-PBEsol bandgap was the unique reported theoretical result for Sr_2CdAs_2 compound; Eg = 0.6 eV, calculated using PAW pseudopotentials 2 (See supporting information).

Optical Properties

Frequency-dependent optical parameters are determined in anenergy range 0-6 eV for incident electromagnetic radiation.

Thermoelectric Properties

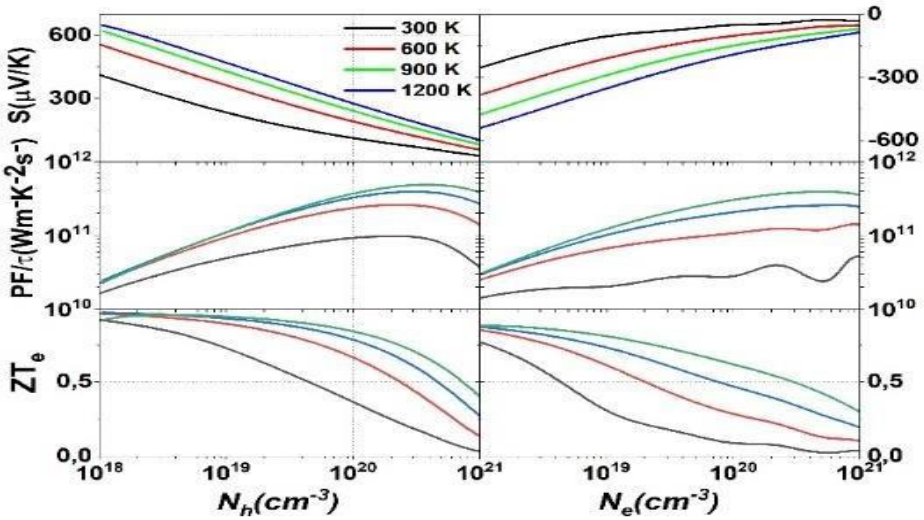

Fig. 2. Transport coefficients of the Seebeck coefficient (S) power factor (PF=$S^2\sigma$) and figure of merit (*ZT*) as a function ofcarrier concentration 10^{18} cm^{-3} and 10^{21} cm^{-3} for the *n*-type and *p*-type doped

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Sr_2CdAs_2 compound at 300, 600, 900 and 1200 K.

According to Fig. 2, we can note the figure of merit ZT reaches amaximum of ~1 for hole concentration of 10^{19} cm^{-3} at 1200k.

Conclusion

In summary, using the FP-LAPW method, it is found that Sr_2CdAs_2 compound is semiconductor with direct band gap at theΓ-point, positioned in the visible sunlight spectrum. Calculated thermoelectric properties proves that p-type title compound is more favorite for thermoelectric performance than the n-type one. Seebeck coefficient of *p*-type title compound of 650 μV/K at 1200 K and the carrier concentration equal to 10^{18} cm^{-3}.

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