Pis'ma v ZhETF, vol. 117, iss. 9, pp. 695 – 696

Insight to structural, electronic, optical and thermoelectric properties of NaCaSb and KCaSb half Heusler compounds: a DFT approach

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Submitted 6 February 2023
Resubmitted 24 March 2023
Accepted 29 March 2023

DOI: 10.31857/S1234567823090094, EDN: bpofse

Due to the necessity for sustainable energy sources, numerous energy conversion technologies have recently been the subject of in-depth research. The transformation of waste heat into productive energy sources have stimulated interest in thermoelectric materials. A figure of merit (ZT) can be used to assess a material suitability for use in thermoelectric (TE) devices expressed as $ZT = S^2\sigma T/\kappa$, where S, σ, T, and κ stand for Seebeck coefficient, electrical conductivity, temperature, and thermal conductivity, respectively [1, 2]. ZT must have a considerable power factor (PF) ($S^2\sigma$) and minimal thermal conductivity (κ) for the best performance. The analysis of these material transport properties was therefore the focus of various theoretical and experimental studies. Using the first principle computing, numerous groups have described the optoelectronic and transport properties of the non-magnetic half heuslers (HHs). Those with eight-valence electrons are expected to have semiconductor properties. Such HHs may have a wide bandgap dependent on the constituent atoms [3, 4]. Zhang et al. recently studied a number of HHs such as CuLiS, KZnS, KBeN, KBaSb, LiMgSb, KInSn including NaCaSb and KCaSb promising for energy harvesting application [5]. P. S. Kacimi et al. explored HHs of type I-II-V and I-III-IV were specifically, their structural, optoelectronic, and transport properties [6]. The outcomes mentioned above inspired us to study further HH compounds. Here, we use first principles simulations to investigate the structural, electrical, elastic, optical, and thermoelectric features of NaCaSb and KCaSb HH compounds. The findings of this study ought to be beneficial for future theoretical and experimental research on HHs. The HHs are found to crystallize in the non-centrosymmetric cubic space group 216, F-43m. To establish if the examined HHs are dynamically stable, we look at the phonon dispersion. The lack of any negative (imaginary) frequencies in the phonon dispersion curves indicates the dynamic stability of the investigated HHs. We estimated the band structures of NaCaSb and KCaSb in order to examine and demonstrate the applicability of the considered compounds for electrical devices. The computed band gap is observed to be indirect for NaCaSb and equals 0.55 and 1.27 eV for generalized gradient approximation (GGA) and modified Becke–Johnson (mBJ) approximation respectively. For KCaSb the computed bandgap is found to be direct and equals 0.49 and 1.23 eV for GGA and mBJ approximation respectively. The variation of the extinction coefficient, $k(\omega)$, in relation to photon energy is investigated. The graph indicates that oscillations are initially undetectable, but as photon energy increases, oscillations can be seen in the visible spectrum. Good absorption spectra facilitate application of the investigated NaCaSb and KCaSb in optoelectronics devices.

For the optimal thermoelectric performance, the Seebeck coefficient must be high. For p-type materials, S is positive, for n-type materials, S is negative. Figure 1a represents the variation of S with temperature suggesting p-type behavior with a positive Seebeck coefficient. The magnitude of σ/τ is increasing with temperature reflecting typical semiconducting characteristics as represented in Fig. 1b. The high electrical conductivity of KCaSb is due to the high density of charge carriers. The σ/κ value is found to be in the range of 10^{-5} indicating better electrical conductivity and less thermal conductivity [7]. The PF, which is a function of electrical conductivity, can be used to estimate a thermoelectric efficiency. The computed PF is shown in Fig. 11d of the main text: for NaCaSb and KCaSb, the obtained PF at 900 K is 2.9×10^{11} W/K^{2}ms and 7.1×10^{11} W/K^{2}ms, respectively. We conclude, the compounds can be used in thermoelectric devices because of the high-power factor at high temperatures.

This is an excerpt of the article "Insight to structural, electronic, optical and thermoelectric properties of NaCaSb and KCaSb half Heusler compounds: A DFT

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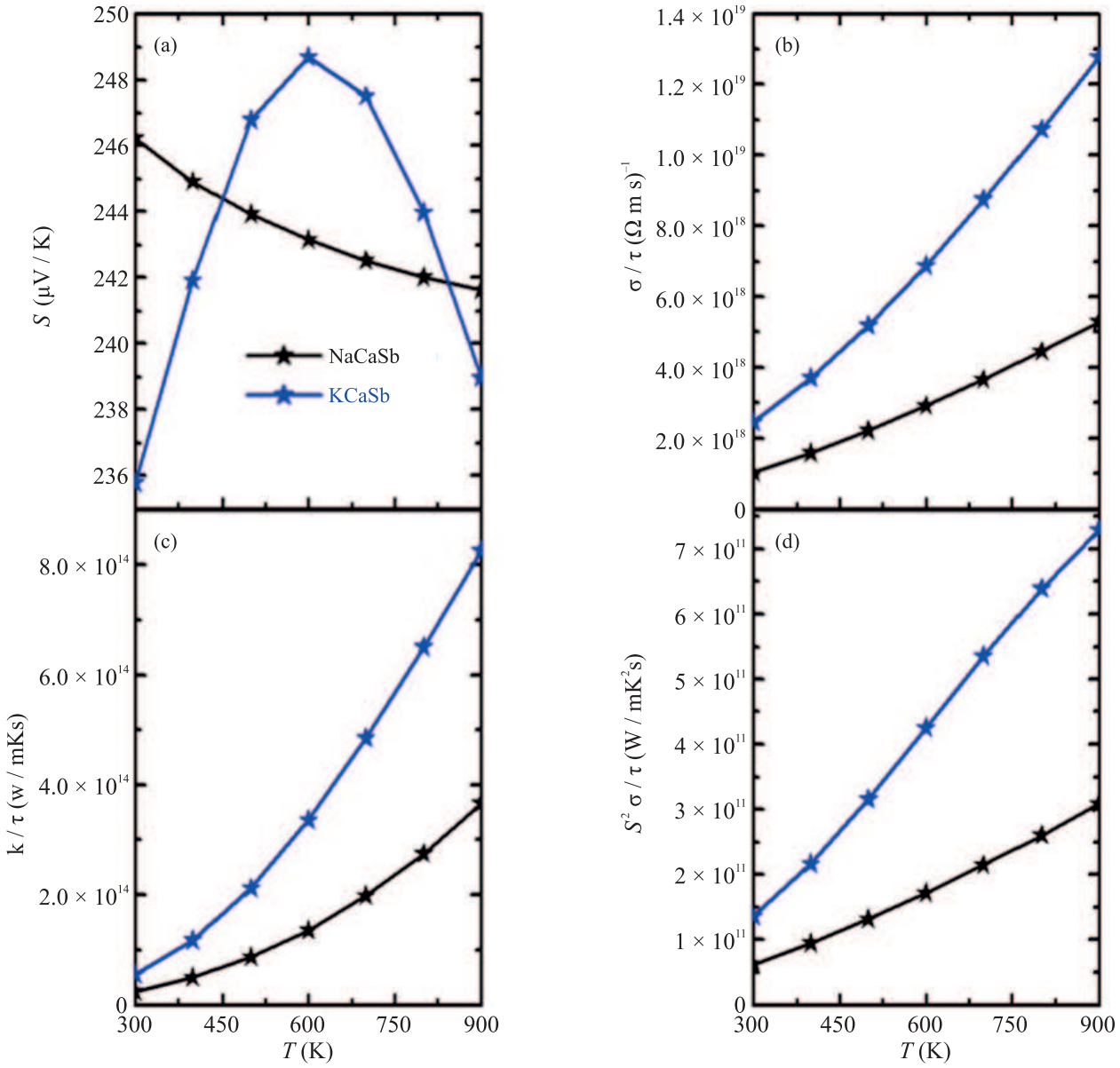

Fig. 1. (Colored online) Computed (a) – Seebeck coefficient S, (b) – electrical conductivity σ/τ, (c) – thermal conductivity κ/τ, and (d) – PF $S^2\sigma/\tau$ for NaCaSb and KCaSb

approach". Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364023600295

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