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A case study of Fe_2TaZ (Z = Al, Ga, In) Heusler alloys: hunt for half-metallic behavior and thermoelectricity

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We have computed the electronic structure and transport properties of Fe_2TaZ (Z = Al, Ga, In) alloys by the full-potential linearized augmented plane wave (FPLAPW) method. The magnetic conduct in accordance with the Slater–Pauling rule classifies them as non-magnetic alloys with total zero magnetic moment. The semiconducting band profile and the density of states in the post DFT treatment are used to estimate the relations among various transport parameters such as Seebeck coefficient, electrical conductivity, thermal conductivity, and figure of merit. The Seebeck coefficient variation and band profiles describe the p-type behavior of charge carriers. The electrical and thermal conductivity plots follow the semiconducting nature of bands along the Fermi level. The overall measurements show that semi-classical Boltzmann transport theory has well-behaved potential in predicting the transport properties of such functional materials, which may find the possibility of their experimental synthesis for future applications in thermoelectric technologies.

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Introduction

Ternary Fe-based Heusler structures constitute a vast family with semiconducting or half-metallic band profiles. These alloys possess excellent properties such as 100% spin polarization, topological phase transition, piezoelectric and thermoelectric power generation, and large curie temperatures.[1–4] Alloys having stabilities w.r.t. temperature, pressure, and exposure to harmful radiations and thus regarded as potential thermoelectric materials. In thermoelectric materials, temperature gradients are expensed to produce electric current, which possibly attracted the attention of energy conservationists as well as researchers worldwide. Hence, to fix the parameters for the performance of thermoelectric materials in a simple way, the figure of merit (zT) has become a handy tool for researchers.

$$zT = \frac{S^2\sigma T}{\kappa} \quad (1)$$

where S is the Seebeck coefficient, T is the absolute temperature, σ is the electrical conductivity, and κ is the total thermal conductivity.[5,6] Mathematically discussing this relation, we can argue that a good thermoelectric material should have a maximum $S^2\sigma$ (called power factor), and a low thermal conductivity κ. It is very difficult to find a suitable material for thermoelectric application with such ideal properties (lower thermal conductivity and higher power factor) because both these quantities are strongly coupled and depend on the crystal structure and electronic properties of a material. DFT has been proved to be a powerful tool to investigate new materials for intriguing properties in a much more adequate way.[7,8] Till date, numerous thermoelectric materials have been investigated; among them, the experimentally proven efficient material is Bi_2Te_3.[9–11] For pure Bi_2Te_3, the highest zT value of 0.7 at 398 K in bulk form was obtained.[12] Presently, Heusler systems[13–15] are being searched for the best possible thermoelectric designs, due to their small lattice and electronic interactions, which consequently minimize the thermal conductivity. ZrCoBi-based half-Heuslers with a record-high zT of ~1.42 at 973 K and a high thermoelectric conversion efficiency of ~9% at the temperature difference of ~500 K were reported recently.[16] Fe_2TiAl has also been found to have thermoelectric applications.[17] Bilc *et al.* reported the room temperature power factors of Fe-based full Heusler alloys, which are 4 to 5 times larger than that of classical thermoelectrics.[18] However, limited information is available on the electronic structure of Fe_2TaZ (Z = Al, Ga, In) alloys. In addition, the untouched bonding parameters and

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