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Inspecting the electronic structure and thermoelectric power factor of novel p-type half-Heuslers

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In line for semiconducting electronic properties, we systematically scrutinize the likely to be grown half-Heusler compounds *XTaZ* (*X = Pd, Pt and Z = Al, Ga, In*) for their stability and thermoelectric properties. The energetically favored *F-43m* configuration of XTaZ alloys at equilibrium lattice constant is a promising non-magnetic semiconductor reflected from its total valence electron count (N_V = 18) and electronic structure calculations. Alongside mechanical stability, the dynamic stability is guaranteed from lattice vibrations and the phonon studies. The energy gaps of these stable Ta-based materials with *Z = Ga* are estimated to reach as high as 0.46 eV when *X = Pd* and 0.95 eV when *X = Pt*; however, this feature is reduced when *Z = Al/In* and *X = Pd/Pt*, respectively. Lattice thermal conductivity calculations are achieved to predict the smallest room temperature value of K_L = 33.6 W/K (PdTaGa) and 38.0 W/mK (for PtAlGa) among the proposed group of Heusler structures. In the end, we investigated the plausible thermoelectric performance of *XTaZ* alloys, which announces a comparable difference for the *n*-type *and p*-type doping regions. Among the six alloys, PtTaAl, PtTaGa and PtTaIn are predicted to be the most efficient materials where the power factor (PF) elevates up to ~ 90.5, 106.7, 106.5 mW/(K^2m), respectively at 900 K; however the lower values are recorded for PdTaAl (~ 66.5), PdTaGa (~ 76.5) and PdTaIn (~ 73.4) alloys. While this reading unlocks avenues for additional assessment of this new class of Half Heuslers, the project approach used here is largely appropriate for possible collection of understandings to realize novel stable materials with potential high temperature applications.

Fast-track discovery of new Heusler semiconductor phases from high-throughput computations and advancement in experimental procedures have endured this giant family to trigger new and active research tactics for potential applications[1–4]. The recent breakthroughs of having superconducting effects[5], high Curie temperatures[6], topological effects like Weyl or Dirac phenomena[7,8], spin varying electronic structure[9,10], skyrmions and giant anomalous Hall effects[11,12] intensified the new paradigm of research on such materials. With the advent of Heusler alloys, practical applications in the device fabrication of spin injectors or magnetic tunnel junctions have gained momentum because of the efficiency and durability[13,14]. Heusler based thermoelectric materials in general have become the spotlight with the recent discovery of a thin layered Heusler material $Fe_2V_{0.8}W_{0.2}Al$ exhibiting a figure of merit (ZT) equal to 5 or 6[15]. The same dimensionless parameter $ZT = S^2\sigma T/\kappa$, governs the efficiency of a thermoelectric module, where Seebeck coefficient (S), electrical conductivity (σ) and thermal conductivity (κ). However, $\kappa = \kappa_e + \kappa_l$ is inturn the sum of electronic (k_e) and phonon (k_l) contribution parts of thermal conductivity[16]. Recently, the artificial layers of Bi_2Te_3 and Sb_2Te_3 displayed the largest values of ZT = 2.4 at room temperature[17]; in SnSe, ZT reached a maximum of 2.6[18], and in p-type PbTe-SrTe, ZT = 2.5[19]. Among Heuslers the TaFeSb[20] and Ti/Sn doped NbFeSb[21] have attained ZT equal to 0.5 and 1.1 experimentally. *Kaur* et al.reported theoretically the p-type semiconductor TiPdSn with 0.74 at 500 K[22] and TaIrSn material with ZT of 0.61 at 900 K[23], which are only few to report amid the vast database of thermoelectric Heuslers. However, efforts are being made to find the more efficient Heusler thermoelectrics to have increased competence in converting waste heat to direct electricity.

Half-Heuslers (HH) possess XYZ-type composition, specifically holding non-centrosymmetric C1b cubic structure[24] within F-43m space group. HH's can be thought as a full-Heusler (FH) X_2YZ structure in which D (0.75, 0.75, 0.75) site is empty and the other three sites, A (0, 0, 0), B (0.25, 0.25, 0.25) and C (0.5, 0.5, 0.5) are occupied by Z, Y and X atoms, respectively in a unit cell. The potential feature of electronic structure of such compounds range from half-metallicity[25] to semiconductor or semimetallic to topological behavior[26,27]. In this article, we examine six half-Heusler compounds with chemical formula XTaZ, where X is (Pd or Pt) atom and Z

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