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Electronic structure and high-temperature properties of doped $Hf_{0.5}Zr_{0.5}CoSb$ phases JACK SIMONSON, SLADE CULP, S. JOSEPH POON, University of Virginia, VIJAYABHARATHI PONNAMBALAM, JUSTINE EDWARDS, TERRY TRITT, Clemson University — Half-Heusler alloys with compositions of the form $Hf_{0.50}Zr_{0.50}CoSb$ were synthesized with Mn substituted to one or both of the Hf/Zr and Co sites or with the Sb site doped with Sn. The thermoelectric properties were evaluated from 300 K to 1000 K. The introduction of Mn was performed to investigate modifications to the band structure near the Fermi energy caused by transition metal substitution. Mn substitutions were discovered to increase the electrical resistivity dramatically while having no beneficial impact upon the thermopower. The Sb-doped alloys, on the other hand, exhibited lowered resistivity and thus increased efficiency of high temperature power generation. The results of both substitutions will be discussed in light of recent first-principles electronic structure calculations. In the Sb-doped alloys, ZT was found to reach 0.5 at 1000 K and is projected to increase to 0.6 K at 1100 K, surpassing the industry standard for p-type materials as set by SiGe alloys.

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