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Effect of doping on the electronic structure and transport properties of half-Heusler compounds[1] MAL-SOON LEE, University of New Orleans, S.D. MAHANTI, Michigan State University, NATHAN J. TAKAS, PARAMATHESH MAJI, FERDINAND P. POUDEU, University of New Orleans —
Narrow-band-gap half-Heusler semiconductors are promising candidates for high-temperature thermoelectrics due to large power factor $S^2\,\sigma$, S is Seebeck coefficient and σ is the electrical conductivity. $S^2\,\sigma$ is usually maximized by changing the carrier concentration through doping. We have carried out transport measurements in $Hf_{0.5}Zr_{0.5}Co_xIr_{1-x}Sb_{0.99}Sn_{0.01}$ for different x and temperatures (T). The nominal hole concentration $n = 1.78 \times 10^{20}/cm^3$. Measured Svalues ($\mu V/K$) are in the range 14-122 at 300 K and 90-216 at 750 K. The systems we have chosen to calculate S are (Hf,Zr)(Co,Ir)Sb. We have used *ab intio* band structure, Boltzmann transport equation (assuming constant relaxation time) and the rigid band approximation (RBA). We find values in the range 121-257 at 300 K and 262-390 at 750 K. To understand the origin of these differences, we have examined the validity of RBA. We observe that isovalent impurities do not change the band structure significantly, whereas charged impurities change the host band structure. Transport properties are also influenced by the change in the band structure.

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