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Electronic and Thermoelectric properties of $RuIn_{3-x}A_x$ (A=Sn, Zn) from first principles[1] DEEPA KASINATHAN, MPI CPfS - Dresden, KLAUS KOEPERNIK, IFW Dresden, HELGE ROSNER, MPI CPfS - Dresden — Recently, substitution derivatives of the intermetallic compound $RuIn_{3-x}A_x$ (A = Sn, Zn) have been shown to exhibit relatively high Seebeck coefficients. Substitution by Sn results in n-type behavior while p-type is the norm for substitution of In by Zn. We discuss in detail the electronic structure of the parent compound and the substitution derivatives obtained from density functional theory (DFT) based calculations using the Full Potential Local Orbital (FPLO) code. The substitution effects have been studied using three different approximations: the simple virtual crystal approximation (VCA), the ordered supercell approach and the disordered coherent potential approximation (CPA). Both Sn and Zn prefer different site symmetry positions in the unit cell. While the parent compound $RuIn_3$ is a semiconductor, the substitution derivatives are not. For small doping concentrations, we observe a rather rigid-band-like behavior due to the parabolic nature of the bands forming the valence band maximum and the conduction band minimum. Transport properties calculated using the semi-classical Boltzmann transport equations (BoltzTraP) based on the constant scattering approximation are consistent with the experiments.

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