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Enhancement of Thermoelectric Properties of Lead Telluride by Doping[1] VLADISLAV O. KONTSEVOI, Illinois Mathematics and Science Academy, JUNG-HWAN SONG, A.J. FREEMAN, Northwestern University — We investigated the effects of doping a promising thermoelectric alloy, PbTe, with a number of mono-, bi- and trivalent dopants, such as Li, Na, In, Tl, As, Sb, Cu, and Zn, by means of first principles calculations using the full-potential linearized augmented plane wave method (FLAPW) with GGA and spin-orbit coupling included. The calculations were performed for 64-atom supercells corresponding to 1.56 at.% doping, and the site preference for dopant atoms was established. We showed that dopant atoms create electronic levels near the band edges that can be beneficial for the improvement of thermoelectric properties. To determine the Seebeck coefficient and the electrical conductivity, we calculated the transport coefficients based on the Boltzmann distribution function in the constant relaxation time approximation, with full intraband optical matrix elements included in the calculation of the group velocity. To calculate the thermoelectric coefficients for different carrier concentrations, the rigid band model was employed. We then explored possible enhancement of the Seebeck coefficient of PbTe in terms of band structure and the electronic density of states at optimal carrier concentrations for certain doping schemes.

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