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Thermoelectric properties of $Yb_{14}MnSb_{11}$ from first-principles[1]

J.-H. SONG, Northwestern U., M. KIM, Ajou U., A.J. FREEMAN, Northwestern U. — The complex Zintl compound, $Yb_{14}MnSb_{11}$, has been recently given much attention as a high-performance thermoelectric due to its nearly twice the figure of metrit (zT) of p-type SiGe at high temperatures ($>$ 900K)[2]. Its high zT can be attributed to low lattice thermal conductivity combined with a large Seebeck coefficient (S) and high electrical conductivity (σ) at high temperatures. To understand the thermoelectric properties of $Yb_{14}MnSb_{11}$ and to find possible improvements for thermoelectric performance, we have investigated its electronic structures and electrical transport properties (S,σ) using the highly precise FLAPW method[3] with the local spin density approximation (LSDA) and LSDA+U[4] methods. We have found significantly different spin moments of Mn between the LSDA and the LSDA+U methods. Also, we determined the anisotropy of the conductivity. The linear temperature behavior of the Seebeck coefficients will be discussed from and related to the electronic structures.

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