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 merit ($zT$) of p-type SiGe at high temperatures ($> 900$K)$^2$. Its high $zT$ can be attributed to low lattice thermal conductivity combined with a large Seebeck coefficient ($S$) and high electrical conductivity ($\sigma$) 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 ($S, \sigma$) 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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