First-principels study of anomalous thermoelectric effect on magnetic materials

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Anomalous transport properties originated in Berry curvature is one of the key ingredients of new thermoelectric(TE) materials. For example, the anomalous Nernst effect (ANE), which is induced by the anomalous Hall effect (AHE) is one of the TE phenomena caused by the Berry curvature. ANE and AHE are reported in various magnetic materials[1, 2] which are not only ferromagnetic but also antiferromagnetic. However the magnitude of anomalous Nernst coefficient is quite small to apply it for TE generation device.

Our aim is to find and design materials with large ANE and clarify the origin of large ANE system. We have investigated two kind of systems as follows based on first-principles calculations based on density functional theory (DFT) implemented in OpenMX code[3]. We have constructed maximally localized Wannier functions (MLWF) using Wannier90 code[4] and evaluated the transport properties within the semiclassical Boltzmann transport theory with relaxation time approximation.

Magnetic half-Heusler compounds CoMSb (M=V, Cr, Mn)

We focused on the half-Heusler compounds CoMSb (M=V, Cr, Mn) and calculated ANE systematically. Half-Heusler intermetallic compounds have a face-centered cubic crystal structure with chemical composition XYZ and space group $F\bar{4}3m$. CoVSb and CoMnSb are known as ferromagnetic compounds with Curie temperatures of 58K and 490K, respectively[5, 6].

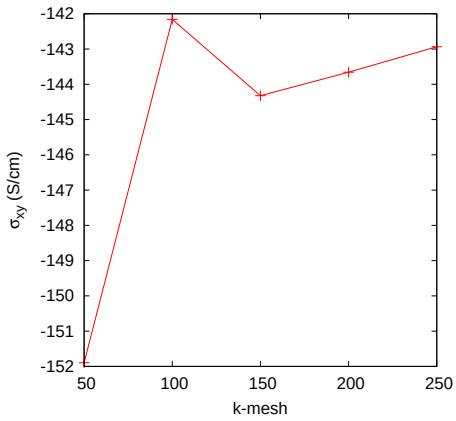

Figure 1: k-mesh dependence of anomalous Hall conductivity $\sigma_{xy}|_{T=0}$ for CoVSb at Fermi energy. σ_{xy} are calculated by using $k \times k \times k$ mesh in the Brillouin zone.

First, we checked the convergence of the anomalous Hall conductivity (AHC) in terms of k point sampling. Figure 1 shows k-mesh dependence of AHC σ_{xy} on CoVSb at Fermi energy. The evaluation of the AHC require a lot of k point sampling and it can be efficiently parallelized. We confirmed that over the 100 k-mesh is sufficient to obtain accurate results.

Figure 2 shows carrier concentration dependence of anomalous Nernst coefficient in CoMSb at 300K. Transport properties are calculated by using constant relaxation time approximation (τ = 3fs). The results show each materials have a peak of ANE near the Fermi energy. We also found that the peaks shift corresponding to the number of valence electron

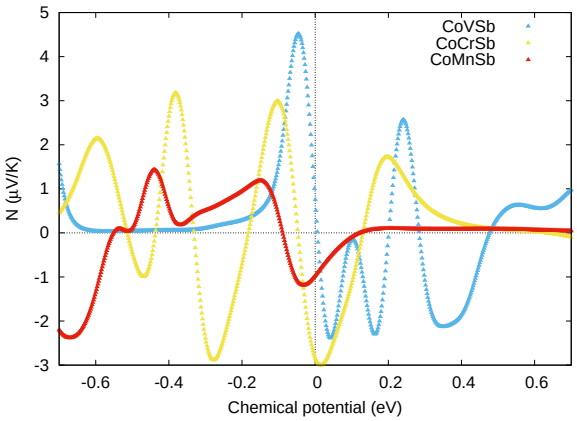

Figure 2: Anomalous Nernst coefficient at 300K. The Fermi energy is set to 0 eV.

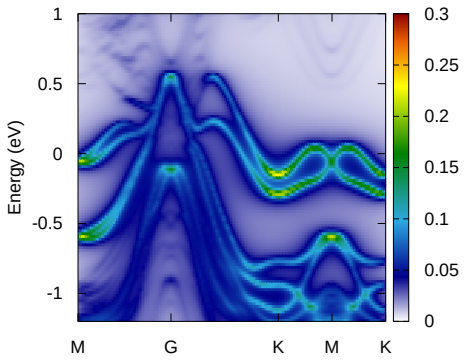

Figure 3: Calculated surface state of Bi-terminated YPtBi. The intensity spectra are calculated by projecting the band onto the 10 atomic-layer unit cell.

of *M*. We investigated CoMnSb in details because of its applicability for an ANE-based TE module that can operate below room temperature. In conclusion, the origin of the large ANE on CoMnSb is the large Berry curvature on symmetry line of the Z-Uz in the Brillouin zone[7].

Topological half-Heusler compound YPtBi

We have calculated topological surface states for half-Heusler compounds YPtBi, which is known as a one of the topological semimetal by using band unfolding method. In this calculation, we used 46 atomic-layer slab model with a vacuum more than 15 Å. The calculation are considered three kind of terminated condition, namely the atom on the surface is Y, Bi, and Pt.

Figure 3 shows calculated surface state of Bi-terminated YPtBi. We obtained non-trivial topological surface sate around the Γ point and metallic surface state around the M point, which is correspond to the calculated and observed results[8].

References

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