Spin Hall conductivity and anomalous Hall conductivity in full Heusler compounds

Yimin Ji1, Wenxu Zhang1,*, Hongbin Zhang2,*, and Wanli Zhang1

1 State Key Laboratory of Electronic Thin Films and Integrated Devices, University of Electronic Science and Technology of China, Chengdu 610054, People’s Republic of China
2 Institute of Materials Science, Technische Universität Darmstadt, Darmstadt 64287, Germany
* Authors to whom any correspondence should be addressed.
E-mail: xwzhang@uestc.edu.cn and hzhang@tu-darmstadt.de

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Abstract
The spin Hall conductivity (SHC) and anomalous Hall conductivity (AHC) in about 120 full Heusler compounds are calculated using the density functional theory in a high-throughput way. The electronic structures are mapped to the Wannier basis and the linear response theory is used to get the conductivity. Our results show that the mechanism under the SHC or AHC cannot be simply related to the valence electron numbers or atomic weights. It is related to the very details of the electronic structures, which can only be obtained by calculations. A high-throughput calculation is efficient to screen out the desired materials. According to our present results, Rh2MnAl and Cu2CoSn, as well as Co2MnAl and Co2MnGa are candidates in spintronic materials regarding their high SHC and AHC values, which can benefit the spin-torque-driven nanodevices.

1. Introduction
Full Heusler compounds with chemical formula X2YZ provide us with an ideal platform to engineer the electronic properties of the materials. The undistorted crystal structure (L2 1 or Cu2MnAl type as defined in the Pearson table) is face-centered cubic with three elements occupying the three different Wyckoff positions: 8c(X), 4a(Y), and 4b(Z) of the space group Fm3m. The X and Y atoms are usually transition metals or lanthanides and the Z sub-lattice is always a main group metal or a semimetal. It has been shown that the compounds can be stable with various combinations of X, Y, and Z elements leading to a tremendous variety of properties attached to them: half metallicity [1], Weyl topological material [2] and thermoelectricity [3–5], etc. The properties can be optimized to meet the special demands in the different areas. For example, the zT can be as huge as 1.5 [6] in the thermoelectric compounds. The half metallicity in Co2YZ, for example, leads to high magnetoresistance, which is crucial in its application in spintronic devices [7, 8]. In the spintronic devices, the spin–orbit coupling (SOC) plays an important role. It is utilized to control spin textures, spin-charge conversions, spin precession, etc. One important way to realize the spin-to-charge conversion is by the spin Hall effect (SHE), which converts a charge current into a spin current, or the inverse SHE (ISHE), which acts oppositely [9]. The key parameter the spin Hall conductivity (SHC) \( \sigma^{\gamma}_{\alpha\beta} \) is written as \( J_\alpha = \sigma^{\gamma}_{\alpha\beta} E_\beta \), where the spin is polarized in the \( \gamma \)-direction and the spin current \( J \) is measured in the \( \alpha \)-direction with the electric field in the \( \beta \)-direction being \( E_\beta \). The SHE stems either from the spin-dependent scattering of defects or the SOC-dependent bands. The latter is a geometrical property of the bands which is named Berry curvature and is intrinsic in solids. Calculations of this intrinsic SHC can be formulated from the linear response theory [10, 11] and the calculated values of Pt, Pd, Au etc [10, 11] are in good agreement with the experiments [12, 13]. In the ferromagnetic compounds, the SOC of the spin polarized conduction electrons gives rise to extraordinary Hall effect called AHE. It was extensively investigated in the magnetic Heusler compounds due to its importance in the spintronics. The pioneer work by Kübler and Felser [14] in the magnetically ordered compounds shows that the strength of SOC can
enhance the AHE under the condition that the other parameters are fixed. The increment comes largely from the X-point in the Brillouin zone (BZ). However, the value in Rh3MnAl is not larger than in Co2MnAl although the heavier element is used. The argument is that the chemical bondings are altered. Giant anomalous Hall effect and Nernst effect in magnetic cubic Heusler compounds were discovered by Noky et al [15, 16]. A high-throughput calculation of the SHC in the 20000 nonmagnetic compounds was recently reported by Zhang et al [17] and a database of the calculated SHC tensors is online. However, the ferromagnetic order does not kill the SHE. The ISHE in the ferromagnetic alloy NiFe was reported by Chien et al [18] about ten years ago. The spin Hall angle was estimated to be the same order as that of Pt. In addition to that, it provides us a way to tune the spin-to-charge conversion efficiency [19–21] by varying the magnetization. Very recently, Leiva et al [22] obtained a giant spin Hall angle of about $-0.19 \pm 0.04$ in the Weyl ferromagnetic Heusler compound Co2MnGa, which is among the highest reported values for a ferromagnet. Regarding to the rapid development of the field, systematic calculations of the SHC and AHC are in demand.

In this work, we calculated the SHC and AHC in the full Heusler compounds from the ICSD database in a high-throughput way. The SHC in the nonmagnetic and ferromagnetic compounds were calculated. We analyze the characteristics of the electronic structures and find that band mixing of the $t_{2g}$ manifold is a key ingredient to obtain large SHC in these compounds.

2. Calculation details

The full Heusler compounds are crystallized in the face-centered-cubic (fcc) structure with the space group of $Fm\bar{3}m$. The compounds were from the ICSD provided by the material project (MP) [23] amounted to about 120. The lattice constant from the database is used in the calculation without optimization. The electronic structure calculations with the fully relativistic treatment of the kinetic energy were performed based on the full potential code [24]. The electronic bands were then projected onto the Wannier functions with the minimum basis sets. The SHC was calculated by the code developed by Železný [25], which evaluates the Kubo’s formula within the linear response theory. The intrinsic SHC can be obtained by computing the spin Berry curvatures [10], which has the following form

$$
\sigma^{\hat{\alpha}\hat{\beta}} = \frac{e}{\hbar} \sum_n \int_{BZ} \frac{d^3 \vec{k}}{(2\pi)^3} J_\alpha^\gamma(\vec{k}) \Omega^\gamma_{n,\alpha\beta}(\vec{k}),
$$

where $\Omega^\gamma_{n,\alpha\beta}(\vec{k})$ is referred as the spin Berry curvature defined as

$$
\Omega^\gamma_{n,\alpha\beta}(\vec{k}) = 2i\hbar^2 \sum_{m \neq n} \frac{\langle u_{m}^{\gamma}(\vec{k}) | J^\alpha_m | u_{n}^{\beta}(\vec{k}) \rangle \langle u_{n}^{\beta}(\vec{k}) | \hat{v}_{\alpha} | u_{m}^{\gamma}(\vec{k}) \rangle}{(\epsilon_n(\vec{k}) - \epsilon_m(\vec{k}))^2},
$$

with $\alpha, \beta, \gamma = x, y, z$ in the Cartesian coordinates, and $m, n$ being the band index. The spin current operator is $J^\gamma_m = \frac{1}{2} \{ \hat{v}_m, \hat{g} \}$, where $\hat{g}_\alpha$ is the spin operator component $\gamma$, and $\hat{v}_\alpha$ is the velocity operator in $\alpha$-direction. The Fermi–Dirac distribution function $f_\alpha(\vec{k})$ is the mean occupation number of the state $(n, \vec{k})$ at a finite temperature $T$. In this work, we set $T = 0 \text{ K}$. As can be seen in equation (1), the temperature dependent in SHC is trivial, which is just the weighted occupation of the states. The variation of SHC can be observed when the large spin Berry curvature is located within $300 \text{ K}$ around the Fermi level. The temperature dependent values of several selected compounds are shown in the supplementary materials (https://stacks.iop.org/NJP/24/053027/mmedia). The third-order tensor $\sigma^{\hat{\alpha}\hat{\beta}}$ represents the spin current $J^\gamma$ generated by an electric field in the $\beta$-direction ($E_3$) via $J^\gamma = \sigma^{\hat{\alpha}\hat{\beta}} E_3$. The spin current is polarized in the $\gamma$-direction and flows in the $\alpha$-direction.

The AHC was calculated similarly, but the spin current operator $J_\alpha^\gamma$ was replaced by the velocity operator $v_\alpha$. In the zeroth-order approximation, the AHE is summation of the spin-resolved Hall conductivity from the spin-up and spin-down channels in ferromagnetic metals. In the ferromagnets, the conductivity tensor is of fourth-order. We calculated the values with the magnetic moment being in the $z$-direction.

The integral over the $k$-space during the calculation of the SHC was sampled in the full BZ with the mesh grids of $200 \times 200 \times 200$ to ensure the convergence with respect to the $k$-mesh. The unit of SHC is $\hbar/e (\Omega^{-1} \text{ cm}^{-1})$. The whole process of the high-throughput calculation is shown in figure 1.

In the cubic crystal, the nonzero elements can be written as $\sigma^{\gamma}_{\alpha\beta} = \sigma^{\gamma}_{\beta\alpha}$, where $\epsilon^{\gamma}_{\alpha\beta}$ is the permutation symbol and $\sigma_0$ is a constant. It is anti-symmetric when $\alpha$ and $\beta$ are interchanged. When the compound is ferromagnetic, we fixed the spin polarization in the $z$-direction and calculated $\sigma^{\gamma}_{xy}$, which means we measure the voltages in the $y$-direction while the spin current is in the $x$-direction.
3. Results and discussions

3.1. SHC and AHC around the Fermi level

The non-zero SHC can be obtained for all the energy levels below and above the Fermi level normally. We can plot the SHC as a function of the Fermi level. However, only the electrons with the energy around the Fermi level are relevant in most spin transport phenomena. We first show the values of $\sigma_{xy}^z$ at the Fermi level. They are plotted with respect to the number of the valence electron, as shown in figure 2(a). The chemical formulas of the compounds with large SHC are shown in the figure. All the data can be found in the supplemented materials. We can see from the figure that the value reaches its maximum when the number of the valence electrons $N_v$ is 26. The largest value in the nonmagnetic compounds is about 400 $\hbar/e(\Omega^{-1} \text{cm}^{-1})$ in Ni$_2$LiSn. In the ferromagnetic compounds, the maximum value is above 700 $\hbar/e(\Omega^{-1} \text{cm}^{-1})$ in Rh$_2$MnAl, with the magnetic moment about 4.08 $\mu_B$/f.u. The magnetic moment projected on Mn is about 3.68 $\mu_B$ in Rh$_2$MnAl. The non-integer magnetic moment indicates the partial filling of the d-orbitals and results in low mobility of conduction electrons. The valence electron number dependent SHC can be partly understood from the electronic structure where the different orbitals are occupied, which will be discussed in the next section. The data show that the values of SHC are all below 2000 $\hbar/e(\Omega^{-1} \text{cm}^{-1})$, which is the value typically obtained in Pt [10]. We see that in the nonmagnetic compounds, for example, the SHC in Ni$_2$LiSn can reach as large as 400 $\hbar/e(\Omega^{-1} \text{cm}^{-1})$, while it is about 600 $\hbar/e(\Omega^{-1} \text{cm}^{-1})$ in the ferromagnetic ordered Co$_2$MnAl and Co$_2$MnGa. The relatively small value of the SHC is rooted in the position of the Fermi level. It is not located at the place where the SOC mixes the states and opens a gap, which can enhance the Berry curvature. Thus the position of the Fermi level is crucial to obtain a large SHC. We noticed that in the experiments by Leiva et al [22], the longitudinal resistivity of Co$_2$MnGa thin film is about 220 $\mu \Omega^{-1} \text{cm}^{-1}$, which is ten times larger than that of Pt thin films. When we account for this much smaller electric conductivity in these compounds [7], the spin Hall angle, which measures the efficiency of the spin to charge conversion efficiency can be comparable with that of noble metals.

The AHC at the Fermi level is shown in figure 2(b). We can see that the maximum of AHC obtained is 1649.21 $\Omega^{-1} \text{cm}^{-1}$ in Rh$_2$MnAl. The same group of the compounds, Co$_2$MnGa, Co$_2$MnAl, and Rh$_2$MnAl can show significantly high AHC and SHC among others with the same $N_v$. The overall distributions of both conductivities with respect to the number of valence electrons are similar. This similarity is rooted in the same mechanism of both effects. In a simplified two-band conducting model, if the spin-non-conserving contributions are overlooked [31, 32], $\sigma_{xy} = \sigma_{xy}^+ + \sigma_{xy}^-$ and $\sigma_{xy} = (\sigma_{xy}^+ - \sigma_{xy}^-) 2h/e$. The relative contributions of the spin channels can be measured by spin polarization $p^H$ of the Hall current written as

$$p^H = \frac{\sigma_{xy}^+ - \sigma_{xy}^-}{\sigma_{xy}^+ + \sigma_{xy}^-}. \quad (3)$$
Figure 2. SHC and AHC at the Fermi level of the Heusler compounds vs the valence electron numbers ($N$). The ferromagnetic and nonmagnetic compounds are denoted with blue and red filled circles, respectively.

Table 1. The magnetic moment ($M$), current polarization ($p^j$), SHC ($\sigma^\uparrow_{xy}$), AHC ($\sigma^\downarrow_{xy}$) and experimental longitudinal conductivity ($\sigma_{exp}^{xx}$) of six selected compounds which show relatively high SHC and AHC.

| Compounds     | $M$ ($\mu_B$/f.u.) | $p^j$ ($A/cm^2$) | $\sigma^\uparrow_{xy}$ ($\Omega^{-1}cm^{-1}$) | $\sigma^\downarrow_{xy}$ ($\Omega^{-1}cm^{-1}$) | $\sigma_{exp}^{xx}$ ($\Omega^{-1}cm^{-1}$) | $\alpha_{SH}$ |
|---------------|--------------------|-------------------|---------------------------------------------|---------------------------------------------|-----------------------------|---------------|
| Rh$_2$MnAl    | 4.08               | 0.87              | 729.1                                       | 1649.2                                      | 1543.7                      | 105.5         |
|               | 4.11$^b$           |                   |                                             |                                             |                             |               |
| Co$_2$MnGa    | 4.09               | 1.01              | 633.1                                       | 1258.9                                      | −1723$^a$, 1500$^b$         |               |
|               | 4.11$^b$, 4.128$^b$|                   |                                             |                                             | −1262.55                    | −3.65         |
| Co$_2$MnAl    | 4.01               | 0.98              | 694.8                                       | 1421.6                                      | 1405.6                      | 16            |
|               | 4.04$^b$, 4.037$^b$|                   |                                             |                                             | 8.5 × 10$^3$                | 0.08          |
| Cu$_2$CoSn    | 1.09               | 1.03              | 578.6                                       | 1119.4                                      | 1138.3                      | −18.9         |
| Co$_2$FeAl    | 5.00               | 0.98              | 29.6                                        | 60.14                                       | 59.67                       | 0.47          |
|               | 5.123              | 55$^f$            | 39$^f$, 40$^f$                              |                                             | 9.6 × 10$^3$                |               |
| Fe$_2$NiGa    | 4.735              | 0.63              | 311.02                                      | 974.54                                      | 798.29                      | 176.25        |
|               |                    |                   |                                             |                                             | 21.0 × 10$^3$               | 0.018         |

$^a$Data from reference [16].
$^b$Data from reference [14].
$^c$Data from reference [32].
$^d$Data from reference [26].
$^e$Experimental data from reference [27].
$^f$Experimental data from reference [28].
$^g$Experimental data from reference [30].
$^h$Experimental data from reference [29].

where $\sigma^\uparrow_{xy}$ and $\sigma^\downarrow_{xy}$ are the spin-up and spin-down Hall conductivities, respectively. We listed the total magnetic moment, spin and Hall current polarization, SHC, and AHC of the five compounds in table 1. The Co-based Heusler compounds were explored by Tung and Guo [32]. Co$_2$MnAl and Co$_2$MnGa were proposed to be used in spintronics due to their simultaneously high AHC and SHC. According to our present results, Cu$_2$CoSn should be added to this material family. We read that except Rh$_2$MnAl, all others show the absolute value of $p^j$ being around 1.0, which means that the SHC is contributed mainly from the spin-up electrons. We noticed the discrepancies in the values reported by the different works. It may come from the slightly different lattice constants we used during the calculations. We use the lattice constants from the ICSD determined by experiments, which also leads to reduction of the magnetic moment.

As mentioned above, the spin-to-charge conversion efficiency is measured by the ratio of the SHC to the longitudinal conductivity, which is known as the spin Hall angle $\alpha_{SH}$. We show the conductivities of four full Heusler compounds in table 1, from which the $\alpha_{SH}$ for these compounds are calculated and shown in...
the table. The largest $\alpha_{\text{SH}} = 0.11$ in Co$_2$MnGa, which is at the same order as that of the intrinsic value of Pt. The compounds with the same $X$ element have similar conductivity, mainly because the DOS at the Fermi level is mainly from the $d$-states of the $X$ element, which shows small dispersion. We can expect that the conductivity of Rh$_2$MnAl and Cu$_2$CoSn are of the same order and lower than that of heavy metals, so that the spin Hall angle can be large.

The data do not show any systematic variation with the atomic numbers, the atomic weights, and the valence numbers which have been explored by us. This is because that the SHC is determined by the mixing of the states due to the SOC, which is dependent on the orbitals and the dispersions alike, as shown in equation (2).

3.2. The electronic structure of the compounds

In order to get insight into the mechanism of the large SHC and AHC, we show the electronic structures of three selected compounds: Ni$_2$LiSn ($N_v = 26$), Cu$_2$NiSn ($N_v = 35$) and Co$_2$MnGa ($N_v = 28$). These compounds have the large SHC among the ones with the same number of valence electrons. The electronic structures of the Heusler compounds from the DFT calculations are well explored in the published literature. The basic characteristics of them can be understood from the molecular orbital model [33], including the crystal field splitting, the bonding of the atoms, and the exchange splittings. For the nonmagnetic cases, it is schematically shown in figure 3, in which we take Ni$_2$LiSn and Cu$_2$NiSn as examples. We group the elements into $X–Y$ and $X–Z$ subgroups. For most compounds, where the $X$ and $Y$ elements are from the TM group, the hybridization of the sp-orbitals from $X$ and main group element $Z$ produces bonding and antibonding $a_1$ and $t_2$ representations of cubic crystal field as shown in figures 3(a) and (b), while those of $d$-orbitals from $X$ and $Y$ form $t_{2g}$ and $e_g$ representations as in figure 3(d). There are non-bonding $d$-orbitals. However, when Li instead of TM elements is at the $Y$ site, ionic bondings are formed due to the large difference in the electron negativity of the elements. There are no additional non-bonding $d$-states. The cases $N_v = 24$ and $N_v = 35$ settle the Fermi level in the $e_g$ and $t_{2g}$ manifold respectively.

We show in figure 4 the electronic bands of the three compounds with relatively high SHC from the ab initio calculations. At the same time, we show the weights from different atomic $d$-orbitals. In Ni$_2$LiSn, as
Figure 4. The electronic band structures of three compounds with projected weights on $dx_z$ and $dy_z$ orbitals are shown. Each of the corresponding SHC is shown on the right panel. In ferromagnetic compound Co$_2$MnGa, the AHC is also shown as in (c).

shown in figure 4(a), the Fermi level is among the $e_g$ states from Ni because of the crystal field as analyzed in the MO orbital model in figure 3(c). The $t_{2g}$ states are located mainly between $-1.0$ eV and $-3.0$ eV. When $Y$ is the TM elements, as Cu$_2$NiSn and Co$_2$MnGa shown in figures 4(b) and (c), the $e_g$ and $t_{2g}$ states from the two subgroups form bonding and antibonding states. The non-bonding $d$-states in Cu$_2$NiSn are around $-3$ eV. The Fermi level crosses the antibonding states from Cu–Ni. It has the $t_{2g}$ characters. The exchange splitting makes the situation a little more complicated. It shifts the occupations of the states in Co$_2$MnGa, as shown in figure 4(c). We see that in Co$_2$MnGa the states near the Fermi level are coming from the 3d states of Mn. It situates at the top of the $t_{2g}$ state of the majority spin and the dip of the states of the minority spins.

3.3. Hints for the large SHC and AHC values
The SHC is a function of the Fermi level. As can be seen in figure 4(a), the maximum of the SHC in Ni$_2$LiSn is about $-1000 \, \hbar/e (\Omega^{-1} \text{ cm}^{-1})$ and locates about 1.8 eV below the Fermi level. We plot the maximum of the SHC absolute values within $\pm 5.0$ eV around the Fermi level achievable in the candidate compounds in figure 5(a). We see that in the figure the maximum is likely to be achieved in the magnetic compounds with $Y = \text{Mn}$ and also in the nonmagnetic Ni$_2$YZ. According to our results in figure 5(a), the SHC in the nonmagnetic compound Ni$_2$CuSn reaches about 1600 $\hbar/e (\Omega^{-1} \text{ cm}^{-1})$. The values in Ni$_2$ScGa and Ni$_2$ScAl are a little bit smaller. We noticed that these compounds contain no heavy elements such as Pt, W, or Bi. However, the SHC can exceed 2200 $\Omega^{-1} \text{ cm}^{-1}$ in Au$_2$MnAl and Pd$_2$MnAl(As) as shown in figure 5(b), which is comparable with that in materials containing these heavy elements. Both AHC and SHC values are plotted as scattered circles filled with different colors for different $Y$ elements as shown in figure 5(c). Generally, a larger AHC also leads to a larger SHC. We fitted the data for $Y = \text{V}$ and Mn respectively. We noticed that when $Y = \text{V}$, the data are less scattered around the linear fitting in green. Due to the near half-metal characteristics observed in the DOS, the spin-non-conserving contributions will be minimized as discussed above. For the other groups of the compounds, the data are much too scattered. The line fitting in red is given just for sight guidance.

It was argued by Banerjee et al that the mixing of the pairs of $\{d_{xz}, d_{yz}\}$ or $\{d_{xy}, d_{x^2−y^2}\}$ orbitals due to the SOC is the main underlying mechanism for the anomalous velocity in TMO [34]. $d_{xy}$ and $d_{x^2−y^2}$ orbitals belong to the different representation basis of the cubic group. According to the molecular orbital picture of the Heusler compounds, the hybridization of the X and Y orbitals forms the $e−t_{2g}$ manifolds, while the orbitals of Z and the second X form the $a_{1g}−t_{2g}$ manifolds due to the cubic symmetry of the crystal field as shown in figures 3(b) and (d). The hybridization of the orbitals with $m = \pm 1$ is possible only within the $t_{2g}$ symmetry. It is anticipated that the Fermi level is located among the $t_{2g}$ manifold in order to obtain a larger effect. Accordingly, for the nonmagnetic compounds, significant SHC can be found in the compounds
when the Fermi level crosses the $t_2$ states or the region when $e_g$ and $t_{2g}$ manifold overlaps with $N_v$ less than 24, or larger than 32. Unfortunately, in quite some Heusler compounds, the Fermi level is located in the gaps formed due to the crystal field [33]. It is not expected that the Fermi level crosses the region of the band mixing, so that the SHC in this case is not large. It is very occasionally that the Fermi level is in the vicinity where the SOC mixes the states and opens a gap. We may conclude that tuning the position of the Fermi level is the key to tuning the SHC. The SHC at the Fermi level is not large, as we argued in the above section, it is due to the position of the Fermi level. When we change the Fermi level, the SHC can be significantly enhanced as shown in figure 4(a). In the nonmagnetic states, the $t_{2g}$ states in Ni$_2$LiSn from Ni $d_{yz}$ and $d_{xz}$ orbitals are located mainly in the energy range between $-1.0$ eV and $-2.0$ eV. It shows very pronounced SHC within the energy window. Hybridizations of the two orbitals occur at the W-point, which is in agreement with the scenario by Jadaun et al [34]. Therefore, as already commented by Kübler et al [14], the AHC is not only determined by the strength of atomic SOC, but also related to the details of the electronic structure, namely, the interactions of the atomic orbitals. From the data obtained so far, we cannot find simple rules to obtain a large SHE in Heusler compounds, although the nodal lines are proposed as a character of the large SHC/AHC [17]. Actually, the values depend on the electronic band structures, and the wave functions as well. We can only figure out the places in the band structures responsible for the SHC/AHC peaks [32]. Thus a high-throughput calculation is the necessary and efficient way to screen out compounds with large SHC and AHC [17].

4. Conclusions

We calculated the SHC and AHC in about 120 full Heusler compounds, both in nonmagnetic and ferromagnetic states. The largest SHC at the Fermi level of nonmagnetic compounds is about $400 \, \hbar/\epsilon$ ($\Omega^{-1} \, \text{cm}^{-1}$) in Ni$_2$LiSn and about $700 \, \hbar/\epsilon$ ($\Omega^{-1} \, \text{cm}^{-1}$) in ferromagnetic Rh$_2$MnAl. The largest AHC is about $1600 \, \Omega^{-1} \, \text{cm}^{-1}$ in Rh$_2$MnAl. These values are significantly larger than the previously proposed Co$_2$YZ compounds. We find that the electronic structure can be well understood from the MO models, where the electronic states formed by the $t_{2g}$ and $e_g$ representations of the cubic symmetry play the determinant role of the properties. It is anticipated that the Fermi level is located among the $t_{2g}$ manifold where the atomic orbitals with quantum number $m = \pm 1$ can be mixed with SOC. Tuning the Fermi level can be a possible way to obtain the high values of AHC or SHC when the largest values are not right at the Fermi level. The Heusler compounds, due to their vast element combinations and varieties of properties, may find more applications in modern spintronic devices.
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Data availability statement

No new data were created or analysed in this study.

ORCID iDs

Hongbin Zhang https://orcid.org/0000-0002-0765-0538

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