Stability of Room Temperature Compensated Half-Metallicity in Cr-based Inverse-Heusler Compounds

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Abstract
Using three correlated band approaches, namely the conventional band approach plus on-site Coulomb repulsion $U$, the modified Becke-Johnson functional, and hybrid functional, we have investigated inverse-Heusler ferrimagnets Cr$_2$CoZ (Z=Al, Ga, In). These approaches commonly indicate that the Cr$_2$CoAl synthesized recently is a precise compensated half-metal (CHM), whereas Cr$_2$CoGa and Cr$_2$CoIn are ferrimagnets with a small moment. This is also confirmed by the fixed spin moment approach. Analysis of the Bader charge decomposition and the radial charge densities indicates that this contrast is due to chemical differences among the Z ions. Additionally, in Cr$_2$CoAl, changing the volume by $\pm$ 5\% or the ratio of $c/a$ by $\pm$ 2\% does not alter the CHM state, suggesting that this state is robust even under application of moderate pressure or strain. Considering the observed high Curie temperature of 750 K, our results suggest that Cr$_2$CoAl is a promising candidate for robust high $T_C$ CHMs. Furthermore, the electronic structure of the CHM Cr$_2$CoAl is discussed.

1. Introduction

The compensated half-metal (CHM), also called the half-metal antiferromagnet,\textsuperscript{1} is a half-metal, which has one metallic and the other insulating spin channels, with the precisely compensated net moment. It is expected that this character have many advantages in spintronics applications which feature zero stray field and high ordering temperatures. Although CHMs have been proposed in diverse crystal structures,\textsuperscript{2} perovskite- or Heusler-related systems have been regarded as the most promising candidates.\textsuperscript{2,3,4,5,6} Recently, Felser and coworkers realized CHM in the Heusler Mn$_3$Ga, in which a small band overlap was observed,\textsuperscript{7} by substitution of some Mn ions with Pt ions.\textsuperscript{8} Kurt et al. also observed the CHM in Ru-doped Mn$_2$Ga thin films.\textsuperscript{9} However, realization of CHM has been very limited and the ordering temperature has remained relatively low.

In this paper, we investigated the inverse-Heusler compounds of the type $X_2YZ$ with a $X - X - Y - Z$ sequence along the diagonal direction in a cubic (the full-Heusler compounds have a $X - Y - X - Z$ sequence), as visualized in the structure of Cr$_2$CoAl shown in Fig. 1. Using the conventional band theory, Meinert and Geisler calculated formation energies and magnetic moments of several inverse-Heusler systems, and predicted the formation of ferrimagnetic states with a tiny moment.\textsuperscript{10} Based on this theoretical suggestion, a few compounds including Cr$_2$CoGa and Cr$_2$CoAl have been synthesized and experimentally investigated. Jamer et al. recently synthesized Cr$_2$CoAl and observed a high Curie temperature $T_C \approx 750$ K,\textsuperscript{11} which was much higher than that in the CHM Mn$_{3-x}$Pt$_x$Ga whose $T_C$ was below 300 K.\textsuperscript{8} The x-ray magnetic circular dichroism measurements indicated a tiny net moment resulting from an antialigned configuration of Cr and Co moments, but due to some impurity phases in the sample it remained unclear whether the net
Table 1: Calculated total and local magnetic moments (in units of \(\mu_B\)) of \(\text{Cr}_2\text{YZ}\) \((Y=\text{Co, Fe; Z=Al, Ga, In, Ge})\), using GGA, +U, +mBJ, and +EECE approaches. Here, GGA+U results are given only for \(U_{\text{eff}} = 3 \text{ eV}\) for Cr and 4 eV for Fe and Co. The CHM character remains unchanged even as the strength of \(U_{\text{eff}}\) is varied in the region of 3 – 5 eV (see text for details). Small values of \(Z\) ions and interstitial contributions in each compound are not given below. For the \(\text{Cr}_2\text{CoIn}\) unsynthesized yet, our optimized lattice parameter, which is similar to the previously reported value, is provided.

| Compounds | Lattice constants (Å) | Experiments | Our calculations | Moments (\(\mu_B\)) | Moments (\(\mu_B\)) |
|-----------|----------------------|-------------|------------------|---------------------|---------------------|
| \(\text{Cr}_2\text{FeGe}\) | \(a = 4.629,\) \(c = 12.414^{[12]}\) | 0.71 GGA | Cr1 Cr2 Y total | -2.38 1.95 2.08 1.4 | +U -2.21 1.73 1.7 0.97 |
|           |                      |             |                  | +mBJ -2.98 2.01 2.21 0.79 | +EECE -3.04 2.25 3.17 2.09 |
| \(\text{Cr}_2\text{CoGa}\) | \(a = 5.79^{[13, 14]}\) \(\sim 320\) 0.26 – 0.31 GGA | Cr1 Cr2 Y | -1.9 1.68 0.42 0.07 | -1.9 1.15 0.97 0.00 | -2.35 1.68 1.0 0.04 |
|           |                      |             |                  | +mBJ -3.02 2.08 1.36 0.06 | +EECE -3.02 2.08 1.36 0.06 |
| \(\text{Cr}_2\text{CoIn}\) | \(a = 5.990\) | 440 – 750 0.21 – 0.46 GGA | Cr1 Cr2 Y | -1.6 1.44 0.34 0.07 | -1.6 0.97 0.82 0.00 |
|           |                      |             |                  | +U -2.14 1.54 0.9 0.04 | +mBJ -2.87 1.98 1.27 0.04 |
|           |                      |             |                  | +EECE -3.44 2.14 0.58 0.13 | +EECE -3.24 2.49 1.54 0.32 |
| \(\text{Cr}_2\text{CoAl}\) | \(a = 5.794^{[11]}\) 750 low-moment GGA | Cr1 Cr2 Y | -1.76 1.59 0.33 0.01 | -1.75 1.15 0.85 0.00 | -2.12 1.65 0.77 0.00 |
|           |                      |             |                  | +U -2.96 2.16 1.23 0.00 | +mBJ -2.96 2.16 1.23 0.00 |

moment was tiny or exactly zero. Additionally, several research groups have observed that the magnetic moment in \(\text{Cr}_2\text{CoGa}\), a promising CHM candidate with high \(T_C\), is very sensitive to the synthesizing conditions.\([12, 13, 14, 15]\) It may be due to antisite disorder, which often occurs in the Heusler compounds. These findings necessitate a fine \textit{ab initio} calculation, including correlation effects not considered previously but which are often crucial in transition metal compounds, to clarify the magnetic ground states. Besides, for further experimental researches it will be useful to investigate how the CHM state is robust under external conditions such as strain and pressure.

Here, we performed fine \textit{ab initio} calculations with very dense \(k\)-meshes, using correlated band theories of the generalized gradient approximation plus \(U\) \((\text{GGA}+\text{U})\),\([16]\) the Tran and Blaha modified Becke-Johnson functional \((\text{mBJ})\),\([17, 18]\) and the hybrid functional\([19]\). Our results indicate that \(\text{Cr}_2\text{CoAl}\) is the most promising candidate of an exact CHM, which is also affirmed by the fixed spin moment approach.\([20]\) We also investigate the stability of this state under pressure or strain. Moreover, we address the electronic structure of the CHM state, which is not reported till now.

2. Structure and calculation

In the cubic inverse Heusler \(X_2YZ\) structure \((\text{space group: } F\bar{4}3m, \text{No. } 216)\), two types of \(X\) ions lie at 4\(a\) \((0,0,0)\) and 4\(c\) \((\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\). The \(Y\) and \(Z\) ions lie at 4\(b\) \((\frac{1}{2}, \frac{1}{2}, 0)\) and 4\(d\) \((\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\), respectively. Some of the inverse Heusler compounds, such as \(\text{Cr}_2\text{FeGe}\) and \(\text{Cr}_2\text{CoGe}\), show a tetragonal distortion. In the tetragonal structure \((\text{space group: } I\bar{4}m2, \text{No. } 119)\), \(X\) ions lie at 2\(b\) \((0, 0, \frac{1}{2})\) and 2\(d\) \((0, 0, \frac{1}{2})\) and the \(Y\) and \(Z\) ions at 2\(a\) \((0, 0, 0)\) and 2\(c\) \((0, \frac{1}{2}, \frac{1}{2})\), respectively. The lattice parameters used in this study are given in Table I. For all compounds, experimentally obtained values were used in our calculations, except for \(\text{Cr}_2\text{CoIn}\) which has not been synthesized yet. Note that our optimized parameters were found to be within 3.5% of the experimental values, so that very little deviation occurred in the magnetic properties.

Our calculations were carried out with the Perdew-Burke-Ernzerhof GGA as the exchange-correlation functional,\([21]\) implemented in the accurate all-electron full-potential code \textsc{wien2k} \([22, 23]\). Correlation effects in the GGA+U approach were treated by the around mean field double-counting scheme,\([16]\) which is often proper for the moderate correlated systems such as the present systems.\([24]\) In these calculations, we varied the effective on-site Coulomb repulsion parameter \(U_{\text{eff}} = U - J\) in the range of 3 – 5 eV for the Cr, Fe, and Co ions, as commonly applied.\([25]\)
Here, $J$ is an intra exchange integral. Additionally, two other correlated band approaches of the hybrid functional and the mBJ, implemented in wien2k, were used to confirm our GGA+U results. In the hybrid functional approach, the exact exchange for correlated electrons functional (EECE) for treating correlated electron systems was chosen with a common 25% of local density exchange replaced by the exact on-site exchange. All results obtained here are very consistent, although there are subtle differences in some cases. As expected, spin-orbit coupling was excluded, since our preliminary calculations showed negligible effects due to this in these systems.

In the wien2k, the basis was determined by $R_{\text{mt}}K_{\text{max}} = 7$ and the augmented atomic radii of $2.28 - 2.5$ a.u. for $X$ and $Y$ ions and $2.18 - 2.39$ a.u. for $Z$ ions. A very dense $k$-mesh containing up to $30 \times 30 \times 30$ points was used to check the convergence of the tiny moment character as a more careful treatment was required near the Fermi level $E_F$.

3. Results

3.1. Magnetic states in the correlated region

Recently, several ferrimagnetic (FI), transition metal-based inverse-Heusler compounds with low moments have been synthesized or theoretically proposed. However, as mentioned in the section of Introduction, the low moment character remains ambiguous. In the experimental point of view, the observed moments are very sensitive to the experimental conditions. In the theoretical point of view, the correlation effects usually relevant to transition metal based compounds have been excluded in the existing calculations. We now investigate these compounds through fine calculations, using the three correlated band approaches based on the density functional theory, with a very dense $k$-mesh. The results are given in Table 1

We first address the tetragonal Cr$_2$FeGe with the observed net moment of $0.71 \ \mu_B$. As a test system to check whether our approaches are reasonable for the Cr-based compounds. The spin of Cr1 ions is antialigned to both the spins of Cr2 and Fe ions, but the moment obtained from GGA is larger than the observed value by a factor of 2.

On the other hand, inclusion of correlation using GGA+U and +mBJ approaches yields very similar moments in the range of $0.79 - 0.97 \ \mu_B$ as those obtained from the experiment. As expected, these results affirm the crucial role of correlation in such Cr-based compounds. Note that the GGA+EECE shows a substantially enhanced moment in Cr$_2$FeGe, whereas in the other compounds studied here the results of all three approaches are very similar.

Next, we investigate the FI Cr$_2$CoGa, which is experimentally the most well-studied among all three so far. Cr$_2$CoGa has both cubic and tetragonal phases with similar magnetic moments. However, the observed Curie temperature $T_C$ (in the range of $440 - 750$ K) and moment $(0.21 - 0.46 \ \mu_B)$ are sensitive to the synthesizing conditions.

Consistently with the experiments, in all our calculations the spin of Cr1 ions is antialigned to both the spins of Cr2 and Co ions, leading to a tiny net moment, but is not exactly compensated. The small moment of Cr$_2$CoGa is negligibly affected by the correlation. So, both experiments and calculations consistently indicate that Cr$_2$CoGa is not an exact CHM.

Figure 2: For Cr$_2$CoAl, change in energy versus fixed spin moment $M$ (in units of $\mu_B$ per formula unit) in GGA and GGA+U. Ferrimagnetic state (FI) is favored over ferromagnetic state (FM) for $M \leq 1.5 \mu_B$, while FM dominates FI for $M \geq 2 \mu_B$. In the shaded region of $1.5 < M < 2.0$, both states coexist. The symbol * denotes the energy of the nonmagnetic state. Here $U_{\text{eff}} = 3 \ \text{eV}$ for Cr and $4 \ \text{eV}$ for Co are used. $E(0)$ is the energy of the CHM state. Inset: Blowup plots below $M \sim 0.2 \mu_B$, indicating that CHM is the ground state in GGA+U. In the Inset, the energies of GGA are enhanced by a factor of 10 for a better visualization.

3.2. Studies of fixed spin moment of Cr$_2$CoAl

We performed fixed spin moment (FSM) calculations to confirm the CHM character of Cr$_2$CoAl. Figure 2 shows the plot of energy increment $\Delta E = E(M) - E(0)$, relative to the energy $E(0)$ of the CHM state, versus fixed spin moment $M$ in both GGA and GGA+U methods. The
The nonmagnetic state has a higher energy by approximately 100 meV than the CHM energy $E(0)$ as obtained from both GGA and GGA+U. Except for the low moment region, both the GGA and GGA+U results show a similar behavior in which the energy increases monotonically with increase in $M$. The inset of Fig. 2 shows a magnified view of the low moment region where the ground state in GGA appears at $M \approx 0.012\mu_B$, consistent with the self-consistent results. However, in the GGA+U, at the region the energy difference $\Delta E$ linearly increases from the value at $M = 0$. The linear behavior of the energy increment is testimony to the character of CHMs or half-metals.[4]

### 3.3. Effects of pressure and strain on magnetic state

To investigate the impact of pressure and the stability of the CHM state in Cr$_2$CoAl, we first vary the volume by $\pm 5\%$ of the experimental value. Remarkably, the net moment remains unchanged in all correlated calculations within this range of volume, except in the EECE case which showed a tiny moment of less than few hundredths of a $\mu_B$ when the volume was enhanced by more than 3%.

Second, the ratio of in-plane and out-of-plane lattice constants is varied to inspect the effect of strain. A small strain does not lead to changing the moment, but a larger strain by over $\pm 2\%$ induces a tiny moment of about a few thousandths $\mu_B$. This is consistent with the tiny difference in the magnetic moments between the cubic and tetragonal Cr$_2$CoGa. It is worthy to be noted that the magnetic moment of Cr$_2$CoIn also remains nearly unchanged, when compressing the volume by 5% or applying a strain. These results indicate that the magnetic states are very robust under application of pressure or strain.

### 3.4. Identifying differences

These differences among the three Cr-based inverse-Heusler compounds can be clarified in two ways. The difference in ionic sizes of $Z$ atoms leads to structural differences. We first compared band structures with the same functionals of their local magnetic moments in each compound. As shown in Fig. 3 even in the identical structure distinctions among band structures of these three systems are very evident near $E_F$, indicating small effects of structural difference. This suggests that applying pressure is not a useful tool to achieve a CHM state in the system, as mentioned above.

Next, we calculated the Bader charges from the wien2k code, given in Table 2. Remarkably, the Al ion is much more ionic than the Ga and In ions. This is also observed in the radial charge density, which is a more efficient way to analyze differences in ionic charges.[31] As shown in Fig. 4 the charge of the Al ion is distributed more closely to the nucleus than that of the other $Z$ ions. This difference in the charge distribution of $Z$ ions affects the charge distribution of Cr1 and Cr2 ions, resulting in considerable variations of their local magnetic moments in each compound. (See Table 1.) These results confirm that the chemical differences among $Z$ atoms, rather than the structure, lead to
distinctions in the magnetic properties. One may expect to achieve an exact CHM state in Cr$_2$CoGa and Cr$_2$CoIn by some Al-doping, so requiring more research.

3.5. Electronic structures of Cr$_2$CoAl

Finally, we address the electronic structures of the CHM Cr$_2$CoAl in the correlated regime, which were not reported before. There are some distinguishing features of the band structures obtained here by the three different correlated band approaches, but they are very similar to each other as a whole. Therefore, only the GGA+U results are presented here, unless mentioned otherwise.

Consistent with the FSM results, the CHM state is energetically favored over the nonmagnetic state by 100 meV per formula unit. Our trials to obtain a ferromagnetic state are presented here, unless mentioned otherwise.

The spin-resolved band structures of the GGA+U are illustrated in Figs. 5 (a) and (b). As depicted in Fig. 5 (a), Cr$_2$CoAl shows a hybridization feature very similar to what has been earlier discussed in other inverse-Heusler compounds. The $d$ orbitals of Cr1-Co ions lead to $\{t_{2g}, e_g\}$ manifolds and nonbonding $\{t_{1u}, e_u\}$ orbitals. These 10 orbitals are hybridized with the Cr2 $d$ orbitals, resulting in bonding $\{t_{2g}, e_g\}$, antibonding $\{t_{2g}^*, e_g^*\}$, and nonbonding $\{t_{1u}, e_u\}$ manifolds. In the minority channel, an indirect gap of 1 eV appears between the $t_{1u}$ and $e_u$ manifolds. In the majority channel, a mixture of the $t_{1u}$ and $e_u$, separated from the other orbitals, is partially filled, indicating a half-metallic character. Notably, in the metallic channel, a nearly flat band appears to cross over $E_F$ along the $\Gamma - X$ line, as often observed in perovskites without $dd\delta$ hopping. This band leads to two interesting features in the density of states (DOS) and fermiology. As shown in the GGA+U total and atom-resolved DOSs of Fig. 6, $E_F$ pinpoints a pseudogap, resulting in a tiny DOS at $E_F$. As picturized in Fig. 7 (b), rod-like hole Fermi surfaces (FSs) appear along the $X$ to $\Gamma$ line. Additionally, there are $\Gamma$-centered hole and $W$-centered elliptical electron FSs, given in Fig. 7. The presence of the pseudogap close to $E_F$ in the metallic channel may lead to unusual transport phenomena like ultrafast demagnetization.

Although the topological properties are not covered here, it is worthy to be noted that the metallic channel shows remarkable features, seemingly related with topological characters, near the Fermi energy $E_F$. As in the full Heusler Co$_2$MnGa, a crossing between the nearly flat band and two-fold bands appears just below $E_F$ along the $\Gamma - X$ line. (See Fig. 6 (a).) In the Co$_2$MnGa, four-bands involved this crossing lead to a hopf-link semimetallic state. Instead, in the inverse Heusler compounds, this crossing leads to six triple points due to lack of inversion symmetry along the (100) in the BZ, implying another interesting topological character. Recently, Shi et al. also suggested a Weyl semimetallic state in the inverse Heusler FI T$_2$MnAl. These interesting topological properties will be discussed elsewhere.
4. Summary

We have investigated a few Cr-based inverse-Heusler compounds $\text{Cr}_2\text{CoZ}$ ($Z=\text{Al, Ga, In}$) through fine electronic structure calculations based on three correlated band approaches, which have been used widely, in the hope of finding promising candidates for compensated half-metals (CHMs).

In these systems, our results show energetically most favored ferrimagnetic state, in which the spin of one of the two Cr ions is antialigned to that of the other Cr and Co ions. In contrast to the other systems showing small moments, the net moment of $\text{Cr}_2\text{CoAl}$ is precisely compensated. This is also confirmed by the fixed spin moment approach. Through analysis of the radial charge distribution, we show that this distinction is due to chemical differences among the $Z$ ions, implying that a precise CHM state would be also obtained by substitution of Al in $\text{Cr}_2\text{CoGa}$ and $\text{Cr}_2\text{CoIn}$. Our results also suggest that the CHM state of $\text{Cr}_2\text{CoAl}$ is robust under pressure or strain. Therefore, considering the observed high $T_C$, $\text{Cr}_2\text{CoAl}$ would be a promising candidate for robust compensated half-metals with a high $T_C$, requiring more experimental research.

5. Acknowledgments

This research was supported by NRF of Korea Grant No. NRF-2016R1A2B4009579.

6. References

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