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Mini-review of interesting properties in Mn_2CoAl bulk and films

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Heusler compounds exhibit many interesting properties, such as high thermopower, magnetocaloric properties, and even topological insulator states. Heusler Mn_2CoAl alloy has been experimentally and theoretically proposed as a promising spin-gapless semiconductor with novel electronic, magnetic, spintronic, transport, and topological properties. Furthermore, the spin-gapless semiconducting-like behaviors are also predicted in Mn_2CoAl films by measuring the transport and magnetic properties. This mini-review systematically summarizes the interesting properties of Mn_2CoAl bulk and Mn_2CoAl-based films. This mini-review is hoped to guide further experimental investigations and applications in the particular scientific community.

KEYWORDS

Mn_2CoAl, spin-gapless materials, Heusler, DFT, density functional theory, film, substrate system

Introduction

On the one side, in 2008, Liu et al. (2008) investigated the structural, electronic, and magnetic properties of Mn_2CoZ (Z = Al, Si, Ge, Sn, and Sb) alloys with Hg_2CuTi-type structure with the help of first-principles calculations, and they stated that all the Mn_2CoZ alloys belong to ferrimagnetic half-metals (Fang et al., 2002; Dowben and Skomski, 2004; Müller et al., 2009; Ashton et al., 2017). It is noteworthy that the spin-gapless semiconducting state of Mn_2CoAl has not been mentioned by Liu et al. (2008). Moreover, Liu et al. (2008) stated that the Mn_2CoZ (Z = Al, Si, Ge, Sn, and Sb) alloys follow the Slater-Pauling rule $M_t = N_V - 24$ (M_t denotes the total magnetic moment and the N_V is the valence electrons in both spin channels). Then, Liu et al. (2008) successfully synthesized the Hg_2CuTi-type Mn_2CoZ alloys, in which the two Mn atoms exhibit different magnetic behaviors. In the same year, Xing et al. (2008) also proposed the half-metallic ferrimagnetism of the Heusler alloys Mn_2CoZ (Z = Al, Ga, Si, Ge) using the first-principles plane-wave pseudopotential method. Moreover, they (Xing et al., 2008) pointed out that the half-metallic states in Mn_2CoZ can maintain in a large range of lattice constants, reflecting robust half-metallic behaviors. In 2011, Meinert, Schmalhorst, and Reiss (Meinert et al., 2011) studied the complex magnetic interactions between the constituents and the Curie temperatures using first-principles calculations. Surprisingly, the Curie temperatures of $Mn_2CoAl/Ga/In$ are all above 800 K.

On the other side, in 2008, Wang, (2008) proposed the concept of a spin-gapless semiconductor. The spin-gapless semiconductor is a new class of zero-gap materials. Spin-gapless semiconductors for practical use should feature 1) completely spin polarized carriers; 2) high mobility of carriers; 3) zero or negligibly small excitation energy of electrons from the valence to the conduction band; 4) easy switching between electron and hole modes by tuning the Fermi level, owing to the ambipolar nature of the band gap (For type II spin-gapless semiconductors). Wang, (2008) proposed that by introducing magnetic ions into the parent nonmagnetic gapless compounds, such as $PbPdO_2$, the spin-gapless semiconducting state can appear. Based on his work, a series of spin-gapless semiconductors (Li et al., 2009; Gao et al., 2015; Wang et al., 2016a; Galanakis et al., 2016; Gao et al., 2016; He et al., 2017; Wang, 2017; Deng et al., 2018a; Huang et al., 2019a; Nadeem et al., 2020; Yue et al., 2020; Yang et al., 2021) with parabolic or linear dispersion between energy and momentum are proposed. More interestingly, topological signatures, such as Dirac point and nodal line states, can be found in spin-gapless semiconductors. For example, He et al. (2017) proposed that $NiCl_3$ monolayer is a near-room-temperature Dirac spin-gapless semiconductor when the spin-orbital coupling (SOC) is absent. When SOC is added, it becomes an intrinsic Chern insulator with a large non-trivial band gap of ~24 meV, at which the quantum anomalous Hall effect could be observed. In 2018, Zhang et al. (2018) proposed the nodal ring spin-gapless semiconducting state in a 2D HK lattice *via* first-principle calculations. In 2022, Ding et al. (2022) summarized almost all the predicted nodal ring/line spin-gapless semiconductors in 2D and 3D materials (Guan et al., 2013; Li and Yang, 2013; Ding and Wang, 2015; Wang et al., 2016b; Rasool et al., 2016; Wang et al., 2017c; Liu et al., 2017; Deng et al., 2018b; Wang et al., 2018; Huang et al., 2019b; Wu et al., 2020b; Guo et al., 2020; Li et al., 2021; Wang et al., 2021; Ji et al., 2022; Wu et al., 2022) in the past 3 years. Remarkably, they (Ding et al., 2022) also provided three valuable suggestions for the future theoretical design of nodal ring/line spin-gapless semiconductors. Moreover, some quaternary Heusler SGSs (Bainsla et al., 2015; Rani et al., 2019) have been prepared, and their interesting gapless behavior has been confirmed. For the verification of the spin-gapless semiconducting property, their specific transport behavior has been widely measured and accepted as strong evidence.

In 2013, the spin-gapless semiconducting state in Mn_2CoAl has been experimentally confirmed by Ouardi et al. (2013a) according to the transport behaviors. They reported that Mn_2CoAl with robust spin polarization is a promising material for room-temperature semiconductor spintronics. In this mini-review, the properties of Mn_2CoAl bulk, Mn_2CoAl [001] surface, Mn_2CoAl/GaAs heterostructures, Mn_2CoAl/Ag/Mn_2CoAl current-perpendicular-to-plane spin valves, MgO/Mn_2CoAl/Pd trilayers, and various types of Mn_2CoAl films are reviewed in details. This mini-review aims to provide an improved understanding of the properties for Mn_2CoAl that have been reported in the last 14 years.

Structural, electronic, elastic, and thermodynamic properties for Mn_2CoAl bulk

The crystal structure of the Heusler alloys can be viewed as a cubic structure with four interpenetrating f.c.c. Sublattices A, B, C, D (see Figure 1A). Normally, full-Heusler alloys X_2YZ can host two types of structures (XA and $L2_1$ type structures). As shown in Figure 1A, we exhibited the XA type and $L2_1$ type Mn_2CoAl. MnMnCoAl and MnCoMnAl represent the XA type Mn_2CoAl and $L2_1$ type Mn_2CoAl, respectively. As mentioned above, Liu et al. (2008) have determined that the crystal structure of Heusler Mn_2CoAl should be XA type (i.e., Hg_2CuTi) instead of $L2_1$. We would like to point out that other researchers have widely investigated the competition between XA and $L2_1$ atomic ordering in full Heusler alloys (Wang et al., 2017a; Wang et al., 2017b; Han et al., 2019a; Han et al., 2019b; Wu et al., 2019; Wu et al., 2020a) in recent years.

Based on the determined XA structure, the spin-polarized band structures for Mn_2CoAl are exhibited in Figure 1B. Obviously, in the minority-spin channel, a direct band gap can be found around the Fermi level, whereas, in the majority-spin channel, an indirect zero-band gap can be observed. Note that, such band structures allow for tunable spin transport. Mn_2CoAl hosts a high Curie temperature of ~720 K and a total M_t of 2 μ_B. In 2015, Chen et al. (2015) investigated the spin-gapless semiconducting states and the dynamical stability of Mn_2CoAl, and they found that the spin-gapless semiconducting states and the dynamical stability can maintain with a pressure less than 25 GPa. The calculated elastic modulus, shear modulus, Yong's modulus, and Pugh's ration for Mn_2CoAl under equilibrium lattice constants are 185.778, 77.782, 204.768 GPa, and 2.39, respectively. Moreover, with the help of the quasiharmonic Debye model, the pressure and temperature dependences of normalized volume V/V_0, bulk modulus B, thermal expansivity, Gruneisen parameter, heat capacity, and Debye temperature are evaluated by Chen et al. (2015) for Mn_2CoAl up to 25 GPa. The above-listed data can be viewed as a reference for the follow-up experimental studies.

Conditions for spin-gapless semiconducting behavior in Mn_2CoAl bulk

In 2014, Galanakis et al. (2014) examined the conditions for the spin-gapless semiconducting state in Mn_2CoAl *via* first-

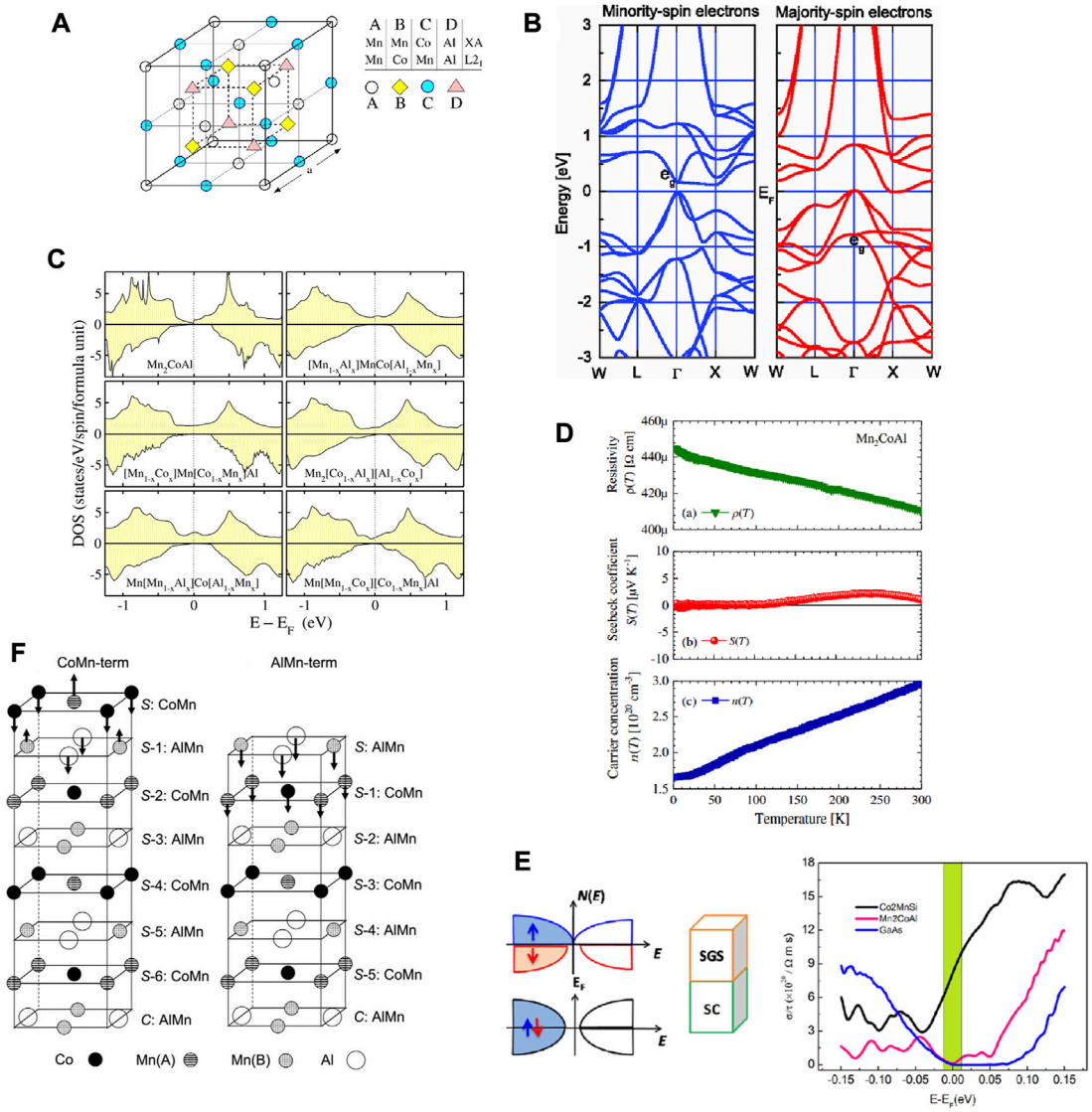

FIGURE 1
(A) Crystal structures of XA and $L2_1$ type Mn_2CoAl. **(B)** Band structures of XA Mn_2CoAl. **(C)** The density of states of Mn_2CoAl by considering atomic swaps. **(D)** Measured resistivity, S(T), and n for Mn_2CoAl sample under different temperatures. **(E)** Schematic diagrams of spin-gapless semiconductor (SGS)/semiconductor (SC) spin injection scheme and the calculated room temperature conductivities for half-metal Co2MnSi, spin-gapless semiconductor Mn_2CoAl, and semiconductor GaAs. **(F)** The (001) Mn_2CoAl surface with Co-Mn and Al-Mn terminated surfaces. Reproduced from Refs. (Ouardi et al., 2013a; Li and Jin, 2013; Galanakis et al., 2014; Xu et al., 2019) with permissions.

principle calculations. They (Galanakis et al., 2014) showed that the spin-gapless semiconducting states in Mn_2CoAl can be kept by applying the tetragonalization of the lattice. However, the spin-gapless semiconducting states in Mn_2CoAl are disappeared by considering the atomic swaps. Swapping the atoms induces a physics nature transition from a spin-gapless semiconducting state to a half-metallic state (as shown in Figure 1C). Furthermore, they (Galanakis et al., 2014) also pointed out that the appearance of Co-surplus will lead to half-metallic states.

Experimentally verified for the spin-gapless semiconducting behavior in Mn_2CoAl bulk

In 2013, the transport measurements of Mn_2CoAl bulk were performed by Ouardi *et al.* (Ouardi et al., 2013b; Ouardi et al., 2019) *via* a physical properties measurement system. They pointed out that Mn_2CoAl bulk hosts a nonmetallic resistivity (see Figure 1D). Note that the resistivity of Mn_2CoAl bulk is two orders of magnitude higher than that of Co_2FeSi metal. From

Figure 1D, one finds that the carrier concentration (n) is temperature independent, and the Seebeck coefficient ($S(T)$) is vanishing. The reason for the appearance of a vanishing $S(T)$ is the compensation of the electron and hole. Note that the temperature-independent n is a main feature for the gapless systems.

Combining the transport and magnetic properties, one can conclude that Mn_2CoAl bulk should be a spin-gapless semiconductor. Ouardi *et al.* (Ouardi et al., 2013b; Ouardi et al., 2019) also reported the magnetoresistance results and the anomalous Hall conductivity of Mn_2CoAl bulk, suggesting Mn_2CoAl is a novel spintronic material.

Note that the transport and magnetic properties cannot be viewed as the only criteria to judge the spin-gapless semiconducting states in Heusler alloys. The microstructure observations (Xu et al., 2019) should also be considered to validate the spin-gapless semiconducting states in Heusler alloys.

New spin injection scheme based on Mn_2CoAl

Spin injection efficiency based on conventional and/or half-metallic ferromagnets/semiconductors is greatly limited by the Schmidt barrier due to conductivity mismatch. In 2015, Xu et al. (2019) proposed that the spin-gapless semiconductor, such as Mn_2CoAl, can be used to replace the conventional and/or half-metallic ferromagnets and form a spin-gapless semiconductor/semiconductor heterostructure (as shown in Figure 1E).

From Figure 1E, we listed the calculated room temperature conductivities for half-metal Co_2MnSi, spin-gapless semiconductor Mn_2CoAl, and semiconductor GaAs. The figure shows that the conductivity of spin-gapless semiconductor Mn_2CoAl is much lower than that of half-metal Co_2MnSi. More importantly, the conductivity of spin-gapless semiconductor Mn_2CoAl is very close to that of semiconductor GaAs. Hence, using spin-gapless semiconductors as the magnetic injectors can reduce the conductive mismatch and enhance the spin injection efficiency.

We would like to point out that the thermodynamic stability, magnetism, and half metallicity of Mn_2CoAl/GaAs (0 0 1) interface have been studied by Feng *et al.* (Feng et al., 2015a) *via* first principle calculations in 2015. In this same year, Feng *et al.* (Feng et al., 2015b) studied the effect of disorder on the electronic and magnetic properties of Mn_2CoAl/GaAs heterostructures from theory.

Electronic structures, magnetism, and half-metallicity for [001] Mn_2CoAl surface

In 2013, Li and Jin (2013) studied the electronic, magnetic, and half-metallic properties of the Mn_2CoAl [001] surface by first-principles calculation. As shown in Figure 1F, two types of surface terminations, i.e., AlMn terminated and CoMn terminated surfaces, are considered by Li and Jin (2013). They Li and Jin (2013) reported that the AlMn-terminated Mn_2CoAl surface hosts half-metallic behavior, whereas the CoMn-terminated Mn_2CoAl surface does not have the half-metallic behavior.

In 2018, Meng *et al.* (Wei et al., 2018) investigated the interfacial electronic, magnetic, and spin transport properties of Mn_2CoAl/Ag/Mn_2CoAl current-perpendicular-to-plane spin valves. Interestingly, they (Wei et al., 2018) pointed out that the $MnCo^T$-terminated interface enjoys the largest interface spin polarization of 78% and magnetoresistance ratio of 2,886%.

Experimental Mn_2CoAl based films

To this date, some investigations are performed on Mn_2CoAl-based films in the experiment. Hence, this section reviews some interesting properties focusing on the Mn_2CoAl-based films. In 2018, Arima et al. (2018) studied the electronic structures and the anomalous Hall conductivity of Si-substituted Mn_2CoAl epitaxial films. Based on the calculated density of states in Figure 2A, one finds that the spin-gapless semiconducting-like behavior can be maintained in $Mn_2CoAl_{1-x}Si_x$ with $x < 0.2$. $Mn_2CoAl_{1-x}Si_x$ films ($0 \le x \le 0.3$) were grown on $MgAl_2O_4$ (100) substrates by molecular beam epitaxy. We collect the θ-2θ x-ray diffraction of the $Mn_2CoAl_{1-x}Si_x$ films in Figure 2B. Arima et al. (2018) stated that the electrical conductivity of $Mn_2CoAl_{0.8}Si_{0.2}$ film is 2340 S/cm, which is closes to that of Mn_2CoAl bulk (2440 S/cm).

In 2013, Jamer et al. (2013) prepared Mn_2CoAl films on GaAs (001) substrates using molecular beam epitaxy. From Figure 2C, one finds the low-temperature resistivity of a 69 nm thick Mn_2CoAl film is about 220 μΩcm, and a metallic-like behavior at low temperatures. They (Jamer et al., 2014) also reported that the Mn_2CoAl films on GaAs (001) substrates exhibited varying amounts of disorder under different annealing temperatures, resulting in the magnetism changing. As the annealing temperature increases, the M_t increases.

In 2014, Xu et al. (2014) prepared Mn_2CoAl films on the thermally oxidized Si substrates by magnetron sputtering deposition. They found that the films host a semiconducting-like resistivity and linear magnetoresistance in the whole region (see Figure 2D). Xu et al. (2014) also reported the unusually low anomalous Hall conductivity, saturation magnetization (1.94 μ_B at 5 K), and the Curie temperature (~550 K). Usually, the results mentioned above are the transport signatures of spin-gapless semiconductors. In 2018, Chen et al. (2018) prepared Mn_2CoAl films on MgO (001) substrates using molecular beam epitaxy. Their electro-

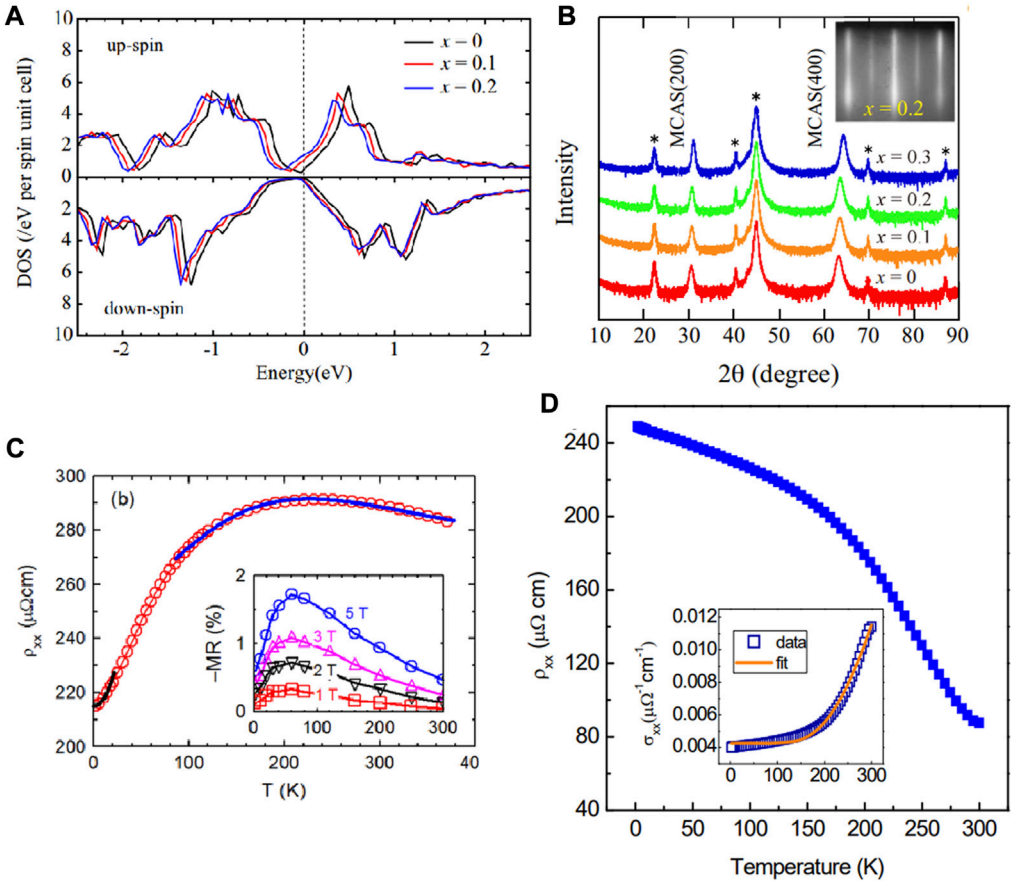

FIGURE 2
(A) Density of states for $Mn_2CoAl_{1-x}Si_x$ (x = 0, 0.1, and 0.2). **(B)** The θ-2θ x-ray diffraction of the $Mn_2CoAl_{1-x}Si_x$ films. **(C)** Resistivity *versus* temperature (red circles). Insert shows magnetoresistance at several magnetic fields. **(D)** The relationship between the resistivity and temperature was measured at zero magnetic fields. The inset shows the fitting of conductivity. Reproduced from Refs. (Jamer et al., 2013; Xu et al., 2014; Arima et al., 2018) with permissions.

and magneto-transport results showed that the Mn_2CoAl hosts spin gapless semiconducting mechanisms at low temperatures. In 2017, Ludbrook and the collaborators (Ludbrook et al., 2017) showed that the MgO/Mn_2CoAl/Pd trilayers could exhibit a novel topological Hall effect in temperatures between 3 K and 280 K. The topological Hall effect is evidence of skyrmions.

Summary

In this mini-review, the electronic, magnetic, and transport properties of Mn_2CoAl bulk, Mn_2CoAl [001] surface, Mn_2CoAl/GaAs heterostructures, Mn_2CoAl/Ag/Mn_2CoAl current-perpendicular-to-plane spin valves, MgO/Mn_2CoAl/Pd trilayers, and various types of Mn_2CoAl films (with $MgAl_2O_4$, GaAs, MgO, and thermally oxidized Si substrates) are reviewed in details. A new spin injection scheme based on Mn_2CoAl and normal semiconductors is also summarized in this mini-review.

Author contributions

The author confirms being the sole contributor of this work and has approved it for publication.

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Conflict of interest

The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

References

Arima, K., Kuroda, F., Yamada, S., Fukushima, T., Oguchi, T., and Hamaya, K. (2018). Anomalous Hall conductivity and electronic structures of Si-substituted Mn2CoAl epitaxial films. *Phys. Rev. B* 97 (5), 054427. doi:10.1103/physrevb.97.054427

Ashton, M., Gluhovic, D., Sinnott, S. B., Guo, J., Stewart, D. A., and Hennig, R. G. (2017). Two-dimensional intrinsic half-metals with large spin gaps. *Nano Lett.* 17 (9), 5251–5257. doi:10.1021/acs.nanolett.7b01367

Bainsla, L., Mallick, A., Raja, M., Nigam, A., Varaprasad, B., Takahashi, Y., et al. (2015). Spin gapless semiconducting behavior in equiatomic quaternary CoFeMnSi Heusler alloy. *Phys. Rev. B* 91, 104408. doi:10.1103/physrevb.91.104408

Chen, P., Gao, C., Chen, G., Mi, K., Liu, M., Zhang, P., et al. (2018). The low-temperature transport properties of Heusler alloy Mn2CoAl. *Appl. Phys. Lett.* 113 (12), 122402. doi:10.1063/1.5046396

Chen, X. R., Zhong, M. M., Feng, Y., Zhou, Y., Yuan, H. K., and Chen, H. (2015). Structural, electronic, elastic, and thermodynamic properties of the spin-gapless semiconducting Mn2CoAl inverse Heusler alloy under pressure. *Phys. Status Solidi B* 252 (12), 2830–2839. doi:10.1002/pssb.201552389

Deng, Y. X., Chen, S. Z., Zeng, Y., Feng, Y., Zhou, W. X., Tang, L. M., et al. (2018). Spin gapless semiconductor and half-metal properties in magnetic penta-hexa-graphene nanotubes. *Org. Electron.* 63, 310–317. doi:10.1016/j.orgel.2018.09.046

Deng, Y. X., Chen, S. Z., Zeng, Y., Feng, Y., Zhou, W. X., Tang, L. M., et al. (2018). Spin gapless semiconductor and half-metal properties in magnetic penta-hexa-graphene nanotubes. *Org. Electron.* 63, 310–317. doi:10.1016/j.orgel.2018.09.046

Ding, G., Wang, J., Chen, H., Zhang, X., and Wang, X. (2022). Investigation of nodal line spin-gapless semiconductors using first-principles calculations. *J. Mat. Chem. C Mat.* 10, 6530–6545. doi:10.1039/d2tc00305h

Ding, Y., and Wang, Y. (2015). Structural, electronic, and magnetic properties of adatom adsorptions on black and blue phosphorene: A first-principles study. *J. Phys. Chem. C* 119 (19), 10610–10622. doi:10.1021/jp5114152

Dowben, P. A., and Skomski, R. (2004). Are half-metallic ferromagnets half metals? *J. Appl. Phys.* 95 (11), 7453–7458. doi:10.1063/1.1682911

Fang, C. M., De Wijs, G. A., and De Groot, R. A. (2002). Spin-polarization in half-metals (invited). *J. Appl. Phys.* 91 (10), 8340–8344. doi:10.1063/1.1452238

Feng, Y., Tian, C. L., Yuan, H. K., Kuang, A. L., and Chen, H. (2015). The effect of disorder on the electronic and magnetic properties of Mn2CoAl/GaAs heterostructures. *J. Phys. D. Appl. Phys.* 48 (44), 445003. doi:10.1088/0022-3727/48/44/445003

Feng, Y., Zhou, T., Chen, X., Yuan, H., and Chen, H. (2015). Thermodynamic stability, magnetism and half metallicity of Mn2CoAl/GaAs (0 0 1) interface. *J. Phys. D. Appl. Phys.* 48 (28), 285302. doi:10.1088/0022-3727/48/28/285302

Galanakis, I., Özdoğan, K., Şaşıoğlu, E., and Blügel, S. (2014). Conditions for spin-gapless semiconducting behavior in Mn2CoAl inverse Heusler compound. *J. Appl. Phys.* 115 (9), 093908. doi:10.1063/1.4867917

Galanakis, I., Özdoğan, K., and Şaşıoğlu, E. (2016). Spin-filter and spin-gapless semiconductors: The case of Heusler compounds. *AIP Adv.* 6 (5), 055606. doi:10.1063/1.4943761

Gao, G., Ding, G., Li, J., Yao, K., Wu, M., and Qian, M. (2016). Monolayer MXenes: Promising half-metals and spin gapless semiconductors. *Nanoscale* 8 (16), 8986–8994. doi:10.1039/c6nr01333c

Gao, Q., Xie, H. H., Li, L., Lei, G., Deng, J. B., and Hu, X. R. (2015). First-principle study on some new spin-gapless semiconductors: The Zr-based quaternary Heusler alloys. *Superlattices Microstruct.* 85, 536–542. doi:10.1016/j.spmi.2015.05.049

Guan, J., Chen, W., Li, Y., Yu, G., Shi, Z., Huang, X., et al. (2013). An effective approach to achieve a spin gapless semiconductor–half-metal–metal transition in zigzag graphene nanoribbons: Attaching A floating induced dipole field via π–π interactions. *Adv. Funct. Mat.* 23 (12), 1507–1518. doi:10.1002/adfm.201201677

Guo, S. D., Mu, W. Q., Zhu, Y. T., and Chen, X. Q. (2020). Coexistence of intrinsic piezoelectricity and ferromagnetism induced by small biaxial strain in septuple-atomic-layer VSi 2 P 4. *Phys. Chem. Chem. Phys.* 22 (48), 28359–28364. doi:10.1039/d0cp05273f

Han, Y., Chen, Z., Kuang, M., Liu, Z., Wang, X., and Wang, X. (2019). 171 scandium-based full heusler compounds: A comprehensive study of competition between XA and L21 atomic ordering. *Results Phys.* 12, 435–446. doi:10.1016/j.rinp.2018.11.079

Han, Y., Wu, M., Feng, Y., Cheng, Z., Lin, T., Yang, T., et al. (2019). Competition between cubic and tetragonal phases in all-*d*-metal heusler alloys, $X_{2-x}Mn_{1+x}V$ (X = Pd, Ni, Pt, Ag, Au, Ir, Co; x = 1, 0): A new potential direction of the heusler family. *IUCrJ* 6 (3), 465–472. doi:10.1107/s2052252519004007

He, J., Li, X., Lyu, P., and Nachtigall, P. (2017). Near-room-temperature chern insulator and Dirac spin-gapless semiconductor: Nickel chloride monolayer. *Nanoscale* 9 (6), 2246–2252. doi:10.1039/c6nr08522a

Huang, H. M., Cao, M. L., Jiang, Z. Y., Xiong, Y. C., Zhang, X., Luo, S. J., et al. (2019). High spin polarization in formamidinium transition metal iodides: First principles prediction of novel half-metals and spin gapless semiconductors. *Phys. Chem. Chem. Phys.* 21 (29), 16213–16222. doi:10.1039/c9cp00958b

Huang, H. M., Cao, M. L., Jiang, Z. Y., Xiong, Y. C., Zhang, X., Luo, S. J., et al. (2019). High spin polarization in formamidinium transition metal iodides: First principles prediction of novel half-metals and spin gapless semiconductors. *Phys. Chem. Chem. Phys.* 21 (29), 16213–16222. doi:10.1039/c9cp00958b

Jamer, M. E., Assaf, B. A., Devakul, T., and Heiman, D. (2013). Magnetic and transport properties of Mn2CoAl oriented films. *Appl. Phys. Lett.* 103 (14), 142403. doi:10.1063/1.4823601

Jamer, M. E., Assaf, B. A., Sterbinsky, G. E., Arena, D. A., and Heiman, D. (2014). Atomic moments in Mn2CoAl thin films analyzed by X-ray magnetic circular dichroism. *J. Appl. Phys.* 116 (21), 213914. doi:10.1063/1.4903771

Ji, Y., Tan, X., Yue, X., Sun, Y., Wang, Y., Liang, H., et al. (2022). Strain-induced spin-gapless semiconductors and pure thermal spin-current in magnetic black arsenic-phosphorus monolayers. *Phys. Chem. Chem. Phys.* 24 (22), 13897–13904. doi:10.1039/d2cp01108e

Li, H., Hayashi, K., Nagashima, Y., Yoshioka, S., Dong, J., Li, J. F., et al. (2021). Effects of disorder on the electronic structure and thermoelectric properties of an inverse full-heusler Mn2CoAl alloy. *Chem. Mat.* 33 (7), 2543–2547. doi:10.1021/acs.chemmater.0c04902

Li, J., and Jin, Y. (2013). Half-metallicity of the inverse heusler alloy Mn2CoAl (0 0 1) surface: A first-principles study. *Appl. Surf. Sci.* 283, 876–880. doi:10.1016/j.apsusc.2013.07.036

Li, X., and Yang, J. (2013). Bipolar magnetic materials for electrical manipulation of spin-polarization orientation. *Phys. Chem. Chem. Phys.* 15 (38), 15793–15801. doi:10.1039/c3cp52623b

Li, Y., Zhou, Z., Shen, P., and Chen, Z. (2009). Spin gapless semiconductor–metal– half-metal properties in nitrogen-doped zigzag graphene nanoribbons. *ACS Nano* 3 (7), 1952–1958. doi:10.1021/nn9003428

Liu, G. D., Dai, X. F., Liu, H. Y., Chen, J. L., Li, Y. X., Xiao, G., et al. (2008). Mn2CoZ(Z=Al, Ga, In, Si, Ge, Sn, Sb)compounds: Structural, electronic, and magnetic properties. *Phys. Rev. B* 77 (1), 014424. doi:10.1103/physrevb.77.014424

Liu, J. H., Kan, X., Amin, B., Gan, L. Y., and Zhao, Y. (2017). Theoretical exploration of the potential applications of Sc-based MXenes. *Phys. Chem. Chem. Phys.* 19 (48), 32253–32261. doi:10.1039/c7cp06224a

Ludbrook, B. M., Dubuis, G., Puichaud, A. H., Ruck, B. J., and Granville, S. (2017). Nucleation and annihilation of skyrmions in Mn2CoAl observed through the topological Hall effect. *Sci. Rep.* 7 (1), 13620. doi:10.1038/s41598-017-13211-8

Meinert, M., Schmalhorst, J. M., and Reiss, G. (2011). Exchange interactions and Curie temperatures of Mn2CoZ compounds. *J. Phys. Condens. Matter* 23 (11), 116005. doi:10.1088/0953-8984/23/11/116005

Müller, G. M., Walowski, J., Djordjevic, M., Miao, G. X., Gupta, A., Ramos, A. V., et al. (2009). Spin polarization in half-metals probed by femtosecond spin excitation. *Nat. Mat.* 8 (1), 56–61. doi:10.1038/nmat2341

Nadeem, M., Hamilton, A. R., Fuhrer, M. S., and Wang, X. (2020). Quantum anomalous Hall effect in magnetic doped topological insulators and ferromagnetic spin-gapless semiconductors—a perspective review. *Small* 16 (42), 1904322. doi:10.1002/smll.201904322

Ouardi, S., Fecher, G. H., Felser, C., and Kübler, J. (2019). Erratum: Realization of spin gapless semiconductors: The heusler compound Mn2CoAl [phys. Rev. Lett. **110**, 100401 (2013)]. *Phys. Rev. Lett.* 122 (5), 059901. doi:10.1103/physrevlett.122.059901

Ouardi, S., Fecher, G. H., Felser, C., and Kübler, J. (2013). Realization of spin gapless semiconductors: The heusler CompoundMn2CoAl. *Phys. Rev. Lett.* 110 (10), 100401. doi:10.1103/physrevlett.110.100401

Ouardi, S., Fecher, G. H., Felser, C., and Kübler, J. (2013). Realization of spin gapless semiconductors: The heusler CompoundMn2CoAl. *Phys. Rev. Lett.* 110 (10), 100401. doi:10.1103/physrevlett.110.100401

Rani, D., EnamullahBainsla, L., Suresh, K., and Alam, A. (2019). Spin-gapless semiconducting nature of Co-rich Co1+xFe1−xCrGa. *Phys. Rev. B* 99, 104429. doi:10.1103/physrevb.99.104429

Rasool, M. N., Hussain, A., Javed, A., Khan, M. A., and Iqbal, F. (2016). Structural stability, electronic and magnetic behaviour of spin-polarized YCoVZ (Z= Si, Ge) and YCoTiZ (Z= Si, Ge) Heusler alloys. *Mater. Chem. Phys.* 183, 524–533. doi:10.1016/j.matchemphys.2016.09.011

Wang, A., Peng, J., Ren, N., Ding, L., Yu, X., Wang, Z., et al. (2021). Spin-gapless states in two-dimensional molecular ferromagnet Fe2 (TCNQ) 2. *J. Phys. Chem. Lett.* 12 (33), 7921–7927. doi:10.1021/acs.jpclett.1c01869

Wang, A., Zhang, X., Feng, Y., and Zhao, M. (2017). Chern insulator and Chern half-metal states in the two-dimensional spin-gapless semiconductor Mn2C6S12. *J. Phys. Chem. Lett.* 8 (16), 3770–3775. doi:10.1021/acs.jpclett.7b01187

Wang, X., Cheng, Z., Wang, J., and Liu, G. (2016). A full spectrum of spintronic properties demonstrated by a C1 b-type Heusler compound Mn 2 Sn subjected to strain engineering. *J. Mat. Chem. C Mat.* 4 (36), 8535–8544. doi:10.1039/c6tc02526a

Wang, X., Cheng, Z., Wang, J., Wang, X. L., and Liu, G. (2016). Recent advances in the Heusler based spin-gapless semiconductors. *J. Mat. Chem. C Mat.* 4 (30), 7176–7192. doi:10.1039/c6tc01343k

Wang, X., Cheng, Z., and Wang, W. (2017). L21 and XA ordering competition in hafnium-based full-heusler alloys Hf2VZ (Z= Al, Ga, In, Tl, Si, Ge, Sn, Pb). *Materials* 10 (10), 1200. doi:10.3390/ma10101200

Wang, X., Cheng, Z., Yuan, H., and Khenata, R. (2017). L2 1 and XA ordering competition in titanium-based full-Heusler alloys. *J. Mat. Chem. C Mat.* 5 (44), 11559–11564. doi:10.1039/c7tc03909c

Wang, X. H., Yang, A. J., Koratkar, N., Chu, J. F., Lv, P. L., Rong, M. Z., et al. (2018). Effects of adatom and gas molecule adsorption on the physical properties of tellurene: A first principles investigation. *Phys. Chem. Chem. Phys.* 20 (6), 4058–4066. doi:10.1039/c7cp07906k

Wang, X. L. (2017). Dirac spin-gapless semiconductors: Promising platforms for massless and dissipationless spintronics and new (quantum) anomalous spin Hall effects. *Natl. Sci. Rev.* 4 (2), 252–257. doi:10.1093/nsr/nww069

Wang, X. L. (2008). Proposal for a new class of materials: Spin gapless semiconductors. *Phys. Rev. Lett.* 100 (15), 156404. doi:10.1103/physrevlett.100.156404

Wei, M. S., Cui, Z., Ruan, X., Zhou, Q. W., Fu, X. Y., Liu, Z. Y., et al. (2018). Interface characterization of current-perpendicular-to-plane spin valves based on spin gapless semiconductor Mn2CoAl. *Appl. Sci.* 8 (8), 1348. doi:10.3390/app8081348

Wu, D. D., Ji, Y. T., Du, G. F., Yue, X. Y., Wang, Y. Y., Li, Q. J., et al. (2022). Spin-gapless semiconducting Cl-intercalated phosphorene bilayer: A perfect candidate material to identify its ferroelectric states by spin-seebeck currents. *J. Mat. Chem. C Mat.* 10 (8), 3188–3195. doi:10.1039/d1tc05932g

Wu, M., Han, Y., Bouhemadou, A., Cheng, Z., Khenata, R., Kuang, M., et al. (2019). Site preference and tetragonal distortion in palladium-rich Heusler alloys. *IUCrJ* 6 (2), 218–225. doi:10.1107/s2052252518017578

Wu, M., Zhou, F., Khenata, R., Kuang, M., and Wang, X. (2020). Phase transition and electronic structures of all-d-metal Heusler-type X2MnTi compounds (X= Pd, Pt, Ag, Au, Cu, and Ni). *Front. Chem.* 8, 546947. doi:10.3389/fchem.2020.546947

Wu, X., Feng, Y., Li, S., Zhang, B., and Gao, G. (2020). 2D Mn2C6Se12 and Mn2C6S6Se6: Intrinsic room-temperature Dirac spin gapless semiconductors and perfect spin transport properties. *J. Phys. Chem. C* 124 (29), 16127–16135. doi:10.1021/acs.jpcc.0c04786

Xing, N., Li, H., Dong, J., Long, R., and Zhang, C. (2008). First-principle prediction of half-metallic ferrimagnetism of the Heusler alloys Mn2CoZ (Z= Al, Ga, Si, Ge) with a high-ordered structure. *Comput. Mater. Sci.* 42 (4), 600–605. doi:10.1016/j.commatsci.2007.09.007

Xu, G. Z., Du, Y., Zhang, X. M., Zhang, H. G., Liu, E. K., Wang, W. H., et al. (2014). Magneto-transport properties of oriented Mn2CoAl films sputtered on thermally oxidized Si substrates. *Appl. Phys. Lett.* 104 (24), 242408. doi:10.1063/1.4884203

Xu, X. D., Chen, Z. X., Sakuraba, Y., Perumal, A., Masuda, K., Kumara, L. S. R., et al. (2019). Microstructure, magnetic and transport properties of a Mn2CoAl Heusler compound. *Acta Mater.* 176, 33–42. doi:10.1016/j.actamat.2019.06.047

Yang, T., Cheng, Z., Wang, X., and Wang, X. L. (2021). Nodal ring spin gapless semiconductor: New member of spintronic materials. *J. Adv. Res.* 28, 43–49. doi:10.1016/j.jare.2020.06.016

Yue, Z., Li, Z., Sang, L., and Wang, X. (2020). Spin-gapless semiconductors. *Small* 16 (31), 1905155. doi:10.1002/smll.201905155

Zhang, L., Zhang, S. F., Ji, W. X., Zhang, C. W., Li, P., Wang, P. J., et al. (2018). Discovery of a novel spin-polarized nodal ring in a two-dimensional HK lattice. *Nanoscale* 10 (44), 20748–20753. doi:10.1039/c8nr05383a