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Editorial: Computational Modeling of Spintronic Materials

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Editorial on the Research Topic

Computational Modeling of Spintronic Materials

In research topic "Computational Modeling of Spintronic Materials", we collected 17 articles dealing with themes as below:

i. Recent advances of spintronic materials;
ii. Frontiers in computational modeling of functional materials.

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Heulser alloys are famous spintronic materials due to they usually host high Curie temperature and adjustable structures. Zhang et al. (Zhang et al., 2020) proposed quaternary Heusler compound CoCrScSn is a half-metal with 100% spin-polarization. Moreover, the elastic constants and half-metallic states under different lattice constants are touched by Zhang et al. Classic Heusler ferromagnets consist of transition-group d-metals and main-group p-elements. As a new direction of Heusler alloy, Wu et al. (Wu et al., 2020) studied a series of all-d-metal Heusler alloys X_2MnTi (X = Pd, Pt, Ag, Au, Cu and Ni). X_2MnTi alloys are without main-group p-elements. Wu et al. also investigated the competition of the cubic $L2_1$ and tetragonal $L1_0$ states of these X_2MnTi alloys. It is hoped that the possible martensitic transformation of these all-d-metal X_2MnTi can be confirmed experimentally.

Half-metals have two spin-directions, one spin channel shows metallic property and the other one features insulating/semiconducting behaviors, resulting in 100% spin-polarization. Also, half-metals can be used for efficient spin injection in spintronics. Doumi et al. (Doumi et al., 2020) proposed that $Ca_{1-x}Cr_xO$ (x = 0.25, 0.5, 0.75) are half-metals, where the ferromagnetism is mainly coming from the direct exchange splitting instead of the crystal field. Deng et al. (Deng et al., 2020) studied the magnetic structure and the Curie temperature of LiMgN with Cu doping, they found that these Cu doped LiMgN systems are dilute magnetic semiconductors with high Curie temperature. More interestingly, $Li(Mg_{0.875}Cu_{0.125})N$ is predicted to be half-metal with a net magnetic moment. Chen et al. (Chen et al., 2020) investigated the electronic structures and magnetism of $Li_{1\pm y}(Mg_{1-x}Cr_x)P$ (x, y = 0.125). They found that Li $(Mg_{0.875}Cr_{0.125})P$ magnet is half-metal.

A series of materials co-exhibiting half-metallic state and topological elements are predicted via first-principles calculations. Chang et al. (Chang et al., 2020) proposed a rhombohedral type $GdMnO_3$ is a half-metal with multiple Dirac-like band crossing points. Li (Li, 2020) proposed $CsCrCl_3$ ferromagnet $P6_3/mmc$ structure is a hypothetical half metal and it also belongs to nodal surface materials. Jia et al. (Jia et al., 2020) reported sandwich-like hexagonal VI_3 monolayer is a half-metal with Weyl fermions. Moreover, a series of topological semimetals and topological metals are reported in the research topic collection: 1) Zhang and Wang (Zhang and Wang, 2020) found that

pure Zr is a topological material with type II nodal line and nodal surface states; 2) Li and Xia (Li and Xia, 2020) reported that cubic HfN is a topological semimetal with zero-dimensional (0-D) and one-dimensional (1-D) topological elements (TEs); 3) Li et al. (Li et al., 2020) proposed that tetragonal PtO is a topological material with nodal point and nodal line states; 4) Xu (Xu, 2020) studied the electronic structures and the topological signatures of XPt (X = Sc, Y, and La) via first-principles calculations. XPt (X = Sc, Y and La) materials are proposed to be novel systems with rich nodal line and nodal point states. Remarkably, we can observe opened and closed nodal lines, and triply degenerate and Dirac nodal points in these systems; 5) Xu et al. (Xu et al., 2020) predicted that hexagonal Zr_3X (X = Al, Ga, In) are metallic systems with high stability and perfect 0-D and 1-D TEs.

Some functional materials and their related physics behaviors are also investigated by first-principles calculations: 1) Ke et al. (Ke et al., 2020) performed a band-gap engineering work to study the band structures and band-gap tailoring of C-mono-doped, C-Ge, and C-Sn co-doped GaN nanosheets; 2) Y_2O_3:Ce magnetic semiconductor with R-3 group symmetry was identified by Ju et al. (Ju et al., 2020) via CALYPSO, and the structural behaviors, doping site locations as well as electronic structures of Y_2O_3:Ce are also studied by Ju et al. via first-principles calculations in details; 3) Yan et al. (Yan et al., 2020) investigated the reaction pathways of H_2 release from the hydrolytic NH_3BH_3 and examined the catalytic roles of small NiCu clusters; 4) Chen et al. (Chen et al., 2020) built an ultrathin van der Waals Fe_3GeTe_2/In_2Se_3 heterostructure and they reported that this heterostructure hosts tunable magnetic anisotropy and Dzyaloshinskii-Moriya Interaction (DMI).

We hope this research topic will attract readers. And we would like to thank all the authors, reviewers and editors who contributed to our research topic.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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