High-Throughput Computational Screening Research on Mn-based Heusler Alloys

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Theoretical Condensed Matter Physics

Clusters
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Software
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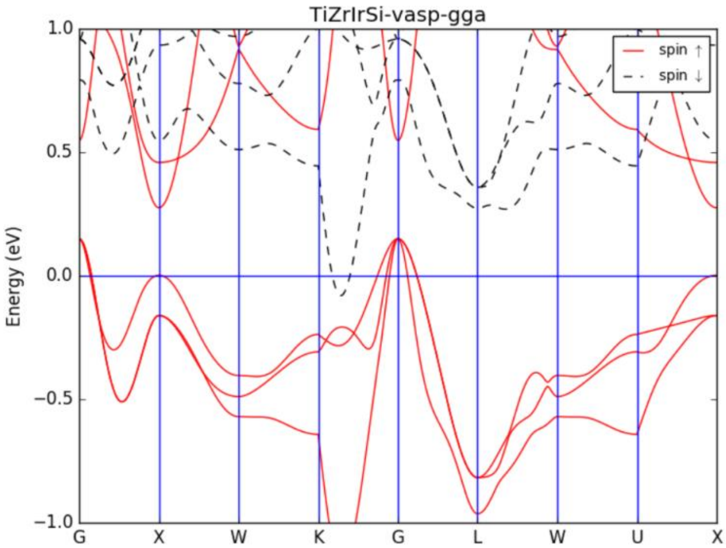

Figure 1: Band structures for TiZrIrSi.

Introduction

Comparing to traditional electronics, spintronics makes use of both charge and spin freedoms of electrons, which is widely applied in high-efficient data storage and transfer. The properties of spin-gapless semiconductors can be easily controlled, making it promising for spintronics design. In the present research, we have done a systemic high-throughput DFT calculations screening for spin-gapless semiconductors in Heusler alloys. We have found 80 new spin-gapless semiconductor candidates.

Methods

The spin-gapless semiconductor which was originally proposed in Co doped $PbPdO_2$ [1] is drawing more and more attention to spintronics community. If the gap in the majority spin channel is zero in a Half metal, then such materials can be classifed as spin-gapless semiconductors. The properties of spin-gapless semiconductors can be easily tunned by shifting the Fermi level. They can be applied in manipulated spintronics.The quaternary Heusler alloy is a good platform for spin-gapless semiconductor research due to various possible components, high Curie temperature and easy synthesise. After years' exploration in quaternary Heusler compounds, an empirical rule has been discovered, that is only with 18, 21, or 26 valence electrons a quaternary Heusler compound can be a spin-gapless semiconductor [2]. According to this rule, there are total about 19,000 possible spin-gapless semiconductor in quaternary Heusler compounds. In order to find more spin-gapless semiconductors, we have done high- throughput density-functional-theory calculation for all the 19,000 possible quaternary Heusler spin-gapless semiconductors.

Results

In our research, we have found 80 new spin-gapless semiconductor candidates. We have shown some new spin-gapless semiconductors among our results in Figure 2. For the shown compoun TiZrIrSi, the valence band maximum and conduction band minimum are in the opposite spin channels. So the carriers will change into the opposite spin channel when they are excited from band maximum to conduction band minimum. We get the conclusion TiZrIrSi can be used for spin switching SGS applications.

Publications

Gao, Q.; Opahle, I.; Zhang, H.: High-throughput screening for spin-gapless semiconductors in quaternary Heusler compounds. Phys. Rev. Materials 3, 024410. https://doi.org/10.1103/PhysRevMaterials.3.024410

Reference

[1] Wang, X. L.: Proposal for a New Class of Materials: Spin Gapless Semiconductors. Phys. Rev. Lett. 100, 156404 (2008). https://doi.org/10.1103/PhysRevLett.100.156404

[2] Wang, X.T. et al.: Recent advances in the Heusler based spin-gapless semiconductors. J. Mater. Chem. C, 4, 7176-7192 (2016) https://doi.org/10.1039/C6TC01343K

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