Jijun Zhao
School of Physics, Dalian University of Technology, Dalian 116024, China
zhaojj@dlut.edu.cn

Computational design of novel 2D electronic and magnetic materials

Abstract
Theoretical design based on first-principles computations play an important role in the research and innovation of 2D materials. In the past few years, our group has designed a series of novel 2D electronic, magnetic and optoelectronic materials: (1) 2D semiconductor with high carrier mobility including monolayer δ-Cu2S [1], GeAsSe, and SnSbTe [2]; (2) Janus group-III chalcogenide monolayers with enhanced piezoelectricity [3]; (3) monolayer group-III monochalcogenides by oxygen functionalization as 2D topological insulators [4]; (2) Y_2N monolayer as high-speed Dirac half-metal [5]; (5) monolayer MnB as 2D ferromagnet with high Curie temperature [6] (see Figure 1).

References

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[2] Y. Guo, et al., Frontier of Physics 13 (2018) 138117
[3] Y. Guo, et al., Appl. Phys. Lett. 110 (2017) 163102.
[4] S. Zhou, et al., npj Quantum Materials 2018, 3, 16
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[6] Z. Jiang, et al., Nanoscale Horizons 3 (2018) 335.

Figures

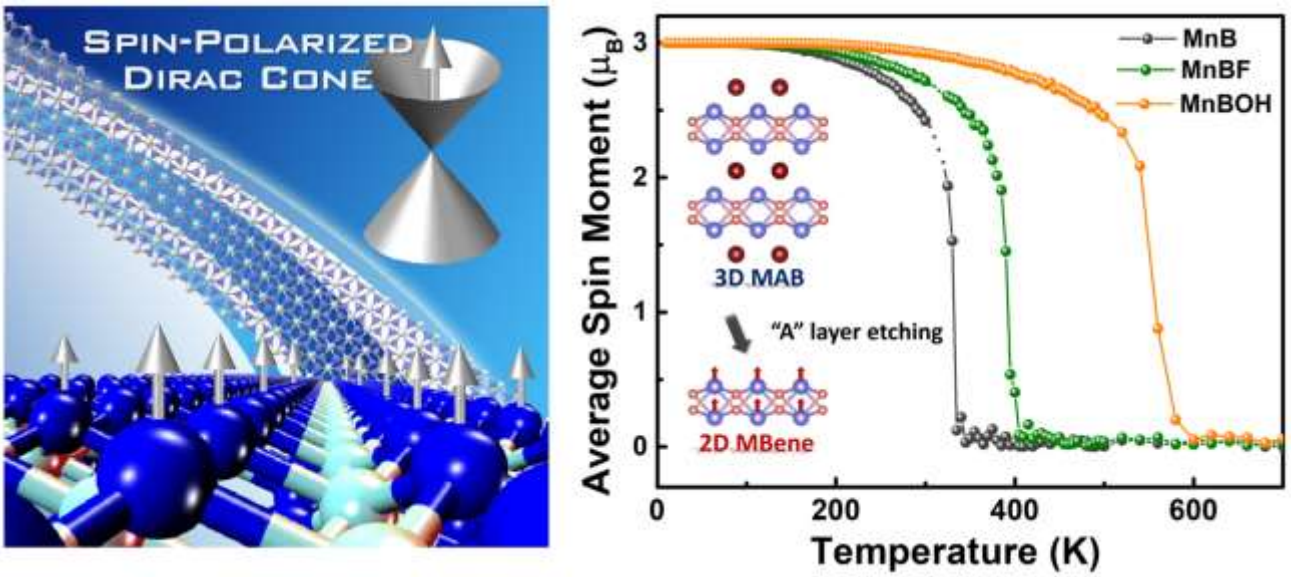

Figure 1: (left) Y_2N monolayer as a Dirac half-metal, (right) monolayer MnB as 2D ferromagnet with high Curie temperature.