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High temperature half-metallicity in 2D $CoGa_2X_4$ (X=S, Se, Te)

The recent discovery of intrinsic ferromagnetic CrI_3 and $Gr_2Ge_2Te_6$ within 70 K creates huge potential for spintronic applications of 2D van der Waals crystals.[1, 2] However, large spin polarization, high phase transition temperature and controllable spin direction are crucial requirements for the spintronic applications of atomically thin magnets. Here, we discover a class of $CoGa_2X_4$ (X= S, Se or Te) monolayer with triangular lattice exhibiting intrinsic half-metallic ferromagnetism. They have large spin gaps in the semiconducting channel, ranging from 2.7 eV for $CoGa_2S_4$ to 1.7 eV for $CoGa_2Te_4$, which makes them stable against the spin flip under weak external disturbances. The magnetocrystalline anisotropy (MAE) calculation with spin-orbital couplingSOC indicates $CoGa_2X_4$ possesses easy plane magnetization, which is expected to have a Berezinskii–Kosterlitz–Thouless transition by classical XY model. The critical temperatures are 886 K, 752 K, and 719 K for $CoGa_2S_4$, $CoGa_2Se_4$ and $CoGa_2Te_4$, respectively. The MAE of $CoGa_2X_4$ are 47 μeV for X=S, 84 μeV for X=Se and 622 μeV for X=Te. The in-plane magnetic moments change to out-of-plane direction if the lattice constants increase from 3.623 Å to 3.75 Å (increase 3.5%), which can be realized through substrate mismatch or other bilayer strain methods. The proposed half-metallic $CoGa_2X_4$ system belongs to the big family of layered AB_2X_4 compounds, which is a significant part of layer-type phases. The stable and steerable magnetization with 100% spin-polarization ratio of $CoGa_2X_4$ would broaden the available design space for spintronics, and connect the magnetic with electronic properties together in 2D materials.

References

[1] Huang, B.; Clark, G.; Navarro-Moratalla, E.; Klein, D. R.; Cheng, R.; Seyler, K. L.; Zhong, D.; Schmidgall, E.; McGuire, M. A.; Cobden, D. H.; Yao, W.; Xiao, D.; Jarillo-Herrero, P.; Xu, X.; *Nature 546* (2017), 270-273.

[2] Gong, C.; Li, L.; Li, Z.; Ji, H.; Stern, A.; Xia, Y.; Cao, T.; Bao, W.; Wang, C.; Wang, Y.; Qiu, Z. Q.; Cava, R. J.; Louie, S. G.; Xia, J.; Zhang, X., *Nature 546* (**2017**), 265-269.

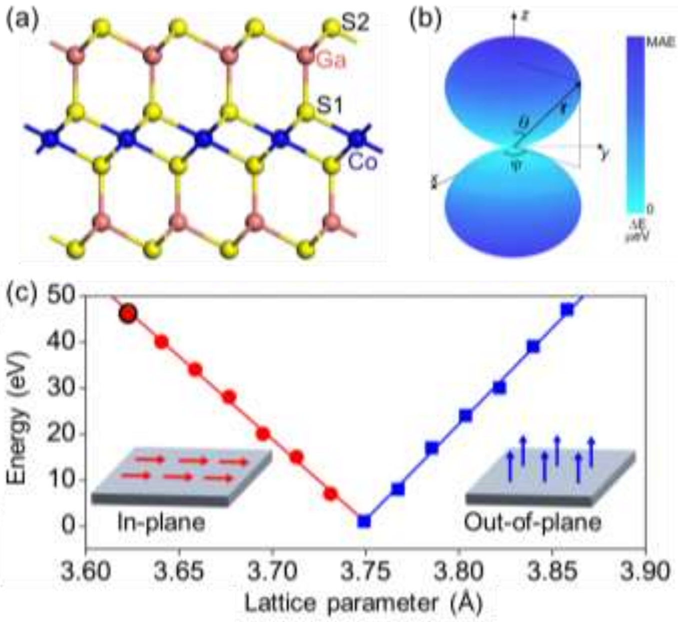

Figure 1: (a) Side view of $CoGa_2X_4$ structure; (b) Schematic map of MAE for $CoGa_2X_4$ monolayer. (c) With the increase of lattice parameters, the in-plane magnetic moments vary to out-of-plane direction.