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Interlayer magnetic coupling in bilayer CrI_3: A first-principles study

Abstract
Recent discoveries of two-dimensional van der Waals (vdW) magnetic materials, especially CrI_3, has accelerated various experimental [1-3] and theoretical [4-6] investigations. It has been shown that CrI_3 has the intriguing interlayer magnetic orderings.: In contrast to the ferromagnetic bulk crystal, a bilayer CrI_3 shows an antiferromagnetic coupling between the layers that is hardly computed as magnetic ground states within conventional first-principles computational methods. In this talk, we show that the spin-dependent vdW interactions and the extended on-site correlation are of vital importance in describing the magnetism in a bilayer CrI_3 within ab initio computation schemes.

References

[1] B. Huang, G. Clark, E. Navarro-Moratalla, Dahlia R. Klein, R. Cheng, Kyle L. Seyler, D. Zhong, E. Schmidgall, Michael A. McGuire, David H. Cobden, W. Yao, Di Xiao, P. Jarillo-Herrero, Xiaodong Xu, Nature, 546 (2017), 270

[2] D. R. Klein, D. MacNeill, J. L. Lado, D. Soriano, E. Navarro-Moratalla, K. Watanabe, T. Taniguchi, S. Manni, P. Canfield, J. Fernández-Rossier, P. Jarillo-Herrero, Science, 6394 (2018), 1218

[3] S. Jiang, L. Li, Z. Wang, Kin Fai Mak, Jie Shan, Nature Nanotechnology, 13 (2018) 549

[4] N. Sivadas, S. Okamoto, Xiaodong Xu, Craig. J. Fennie, and Di Xiao, Nano Letters, 18 (2018), 7658

[5] P. Jiang, C. Wang, D. Chen, Z. Zhong, Z. Yuan, Zhong-Yi Lu, and Wei Ji, Phys. Rev. B, 99 (2019), 144401

[6] S. W. Jang, M. Y. Jeong, H. Yoon, S. Ryee, and M. J. Han, Phys. Rev. Mater., 3 (2019), 031001(R)