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

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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.

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