Interplay between stacking and magnetic configurations in MPS_3 bilayers

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The two-dimensional transition metal thiophosphates MPS_3 (M = Mn, Fe, and Ni) have attracted a lot of attention recently because they exhibit a long-range antiferromagnetic (AFM) order and display interesting electronic-optical properties associated with their magnetic state [1]. In these materials, the AFM ground state is governed by the competition between direct M–M exchange and indirect M–S–M superexchange interactions within atomic layers, as well as the d-electron occupancy of the metal ion [2]. However, how the stacking between layers influences the electronic properties of MPS_3 is largely unknown. Here, we perform first-principles calculations to study the interplay between AFM and ferromagnetic (FM) configurations under different layer stacking (see Figure 1). Our results provide insight into understanding the interlayer AFM-FM coupling in those systems, revealing that different magnetic states can be stabilized through layer stacking. We suggest that these systems provide a unique playground for studying different aspects of magnetism in 2D systems.

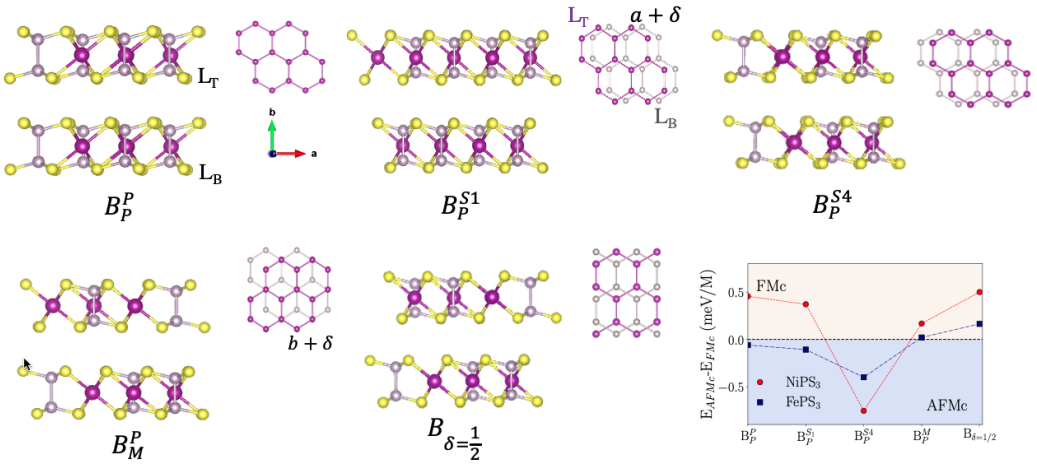

Figure 1. Different high-symmetry stacking configurations in bilayer MPS_3. The top view to the right of each structure indicates the stacking of the two hexagonal lattices of the transition metals. The low-right panel shows the interlayer exchange energy for each stacking.

References

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[2] B. L. Chittari et al., Physical Review B, **94** 184428 (2016).