2D materials are extremely popular due to their unique properties. We are especially interested in 2D magnets. The aim of our research was to study the intralayer and interlayer magnetism in a NiPS$_3$/FePS$_3$ heterostructure. Within NiPS$_3$ and FePS$_3$ monolayers four different spin arrangements were considered. We compared various distances between the NiPS$_3$ and FePS$_3$ layers in heterostructure. For the optimal distance we compared two stackings and two magnetic arrangements.

Abstract

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Computational details

- Ab initio calculations in the framework of density functional theory (DFT)
- Numerical package VASP (Vienna Ab Initio Simulation Package)
- GGA+U approach with Hubbard $U_{Ni} = 6.45$ eV, $U_{Fe} = 5.3$ eV
- Van der Waals correction included (DFT-D3)
- Kinetic Energy cutoff = 400 eV
- K-point grid: 10x6x2
- Slab calculations - vacuum width = 20 Å

Results

Fig. 1. Electronic structure for NiPS$_3$ for different magnetic orders.

Fig. 2. Energy of the NiPS$_3$/FePS$_3$ bilayer with AA stacking versus interlayer distance.

Fig. 3. Electronic structure for NiPS$_3$/FePS$_3$. Different stacking comparison and magnetic order comparison.

Conclusion

- The optimal interlayer distance 3.4 Å is the same for each magnetic order in NiPS$_3$/FePS$_3$ bilayer
- There is a moderate influence of intralayer magnetism on the properties of the system (NiPS$_3$ and FePS$_3$)
- There is a negligible impact of interlayer magnetism on the properties of the system (NiPS$_3$/FePS$_3$)

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