High-throughput stacking reveals emergent and switchable properties of 2D van der Waals bilayers

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Abstract

Stacking atomically thin two-dimensional monolayers into van der Waals (vdW) heterostuctures [1] offer new opportunities to control physical properties of 2D materials. Here we provide a systematic ab initio-based study of homo-bilayers created by stacking several hundreds of stable monolayers containing up to 10 atoms per unit cell. We investigate all configurations commensurate with the primitive unit cell. We further verify the predictive power of our stacking approach by comparing our stacking orders when exfoliable bulk compounds of the same material exist. For the stable bilayers within a 3 meV/A^2 binding energy distance from our most stable configuration, we calculate a range of electronic and magnetic properties. We further explore switchable properties in bilayer pairs where two stable stacking configurations are related with a slide vector. Experimental evidence of switching such bilayers have been recently reported [2, 3]. Our work contributes to the systematisation of 2D materials and represents a step towards rational design of layered vdW materials. Our results will be available online and well-integrated with the Computational 2D Materials Database (C2DB) [4, 5] which allows for comparison between mono- and bilayer properties.

References

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