On van-der-Waals interactions in two-dimensional and layered materials

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ABSTRACT

Van der Waals interactions, more precisely London dispersion, are attractive interactions arising between chemically saturated species. They are the reasons why layered materials do not fall apart into individual sheets of strongly bonded two-dimensional (2D) crystals. The stacking between 2D crystal layers can have different configurations, and somewhat surprisingly, the interlayer interaction has a significant effect on the electronic properties of the bilayers.

In this talk, I will focus on the computational approaches that are available to tackle 2D and layered materials, including London dispersion-corrected density-functional theory [1,2]. I will discuss the impact of symmetry and spin-orbit corrections [3-5]. I will show systems of particularly interesting interlayer interactions, including blue phosphorene, gray arsenene [6] and their mixed phases [7] as well as platinum diselenide, a materias where the stacking can even change the character from semiconducting to metallic [8-10].

References

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