Electronic structure calculations on MX_2 dichalcogenide/Graphene hybrid structures.

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Abstract

Since the first isolation of graphene in 2004 [1] there has been much effort in exploiting its outstanding electronic properties [2] to technological applications, in particular, in combination with other two-dimensional crystals. There have been many studies of the Boron Nitride (BN)/graphene interaction due to the small mismatch between both of them that avoids graphene losing its electronic properties [3].

Nowadays, transition metal dichalcogenides (TMDC) such as MoS_2 and WS_2 are bringing much attention due to the fact that, although in nature they exhibit a bulk structure, they are layered materials which can be exfoliated like graphene to produce 2D single or multi-layer structures [4]. Interestingly, they are semi-conductors with a change in their electronic structure properties when changing from bulk (which presents an indirect gap) to a single layer (with a direct gap). This opens up new possibilities for the creation of new electronic and optoelectronic devices.

The small mismatch between MoS_2 and WS_2 with graphene, also opens a wide possibilty of creating new devices. Recently, two papers by Britnell et al. [5] and Georgiu et al. [6] have shown good performance in FETs fabricated using this MoS_2/graphene and WS_2/graphene hybrid structures.

Here, we present ab-initio DFT calculations (done using the Siesta code [7]) of the electronic properties of single-, multi-layer and bulk MoS_2 and WS2. We also study the interaction of these materials with graphene and the possibility of fabricating new devices with these hybrid structures [4,8]. For this, we first study the interaction of a single layer of MoS_2 or WS_2 with graphene (Fig. 1 and 2). We find the optimal distance between graphene and MoS_2 and WS_2 and show that an interface dipole is created between them. We also find that the electron density distortion is inhomogeneous, following the mismatch between the graphene and WS_2 lattices. Finally, we study the change of this properties when changing the number of layers of MoS_2 and WS_2 in the system.

References

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Figures

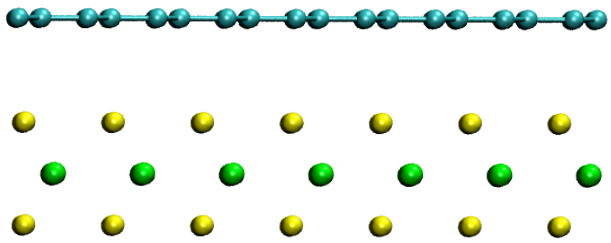

Figure 1: Side view of the TMDC/graphene structure. Carbon is represented in blue, tungsten (molybdenum) in green and sulphur in yellow.

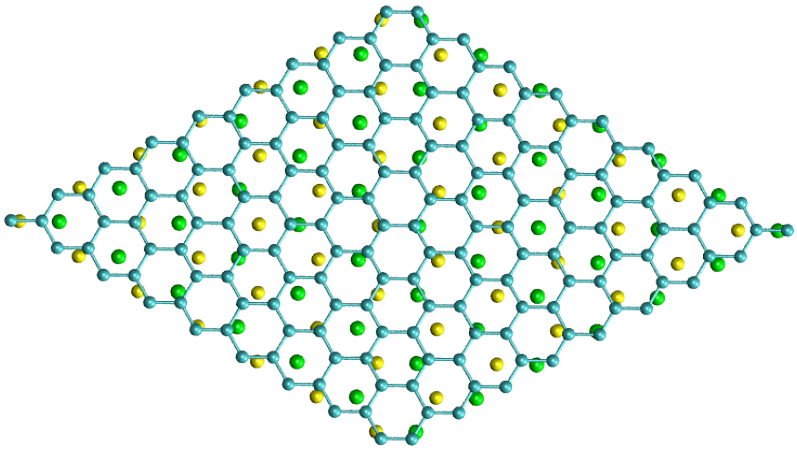

Figure 2: Top view of the TMDC/graphene structure. Carbon is represented in blue, tungsten (molybdenum) in green and sulphur in yellow.