Minimal tight-binding model for transition metal dichalcogenides.

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Abstract

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 [1] (see Fig. 1). 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.

In this work, we try to find the minimal tight-binding model to correctly describe the density functional theory (DFT) bands. That is, the model with the minimum basis and interactions that can adjust to these bands. To do so, we build a model based on the one developed by Capelluti et al. [2] and we add orbitals and nearest neighbours interactions comparing, for each case, the obtained bands with the ones calculated with an ab-initio code (Siesta [3]). We also investigate the effect of the basis overlap in the model.

References

[1] Q. H. Wang, et al., Nature Nanotech. 7, 699 (2012).

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[3] J. M. Soler, et al., Journal of Physics: Condensed Matter 14 , 2745 (2002).

Figures

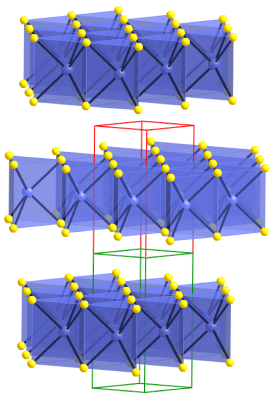

Figure 1: Atomic structure of a transition metal dichalcogenide with a 2H structure such us 2H-MoS_2 or 2H-WS_2. The small green rectangle represents the unit cell of a monolayer. The red extension represents bulk crystal.