Large phosphorene in-plane contraction induced by interlayer interactions in graphene-phosphorene heterostructures

Benoit Van Troeye
Aurélien Lherbier, Jean-Christophe Charlier, Xavier Gonze

Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Chemin des étoiles 8, B-1348 Louvain-la-Neuve, Belgium

benoit.vantroeye@uclouvain.be

Intralayer deformation in van der Waals (vdW) heterostructures is generally assumed to be negligible due to the weak nature of the interactions between the layers, especially when the interfaces are found incoherent. In the present work, graphene-phosphorene vdW-heterostructures (see Figure 1) are investigated with the Density Functional Theory (DFT). The existing degrees of freedom in such systems (rotation angle between the layers, intralayer deformations, etc.) are carefully examined. The alignment of the shared crystalline directions of graphene and phosphorene (zigzag on zigzag) is found favourable energetically, alongside with a ~4% phosphorene contraction along the armchair direction (see Figure 2), and that even in the case of an incoherent interface between graphene and phosphorene.

Furthermore, the possibility of a commensurate coherent interface can not be discriminated from our analysis; the formation of such interface would be accompanied with a change of the character of the phosphorene gap, from direct to indirect. This work highlights thus the possibility of substrate-controlled stresstronics in phosphorene thanks to its small elastic constant along the armchair direction (~20x smaller than graphene, for which coherent interfaces with h-BN can be created experimentally [1]). Finally, several models and tools are presented in order to alleviate to some extent the DFT limitations in the study of vdW-heterostructures.

References

[1] A. Davies, J. D. Albar, A. Summerfield, J. C. Thomas,T. S. Cheng, V. V. Korolkov, E. Stapleton, J. Wrigley, N. L. Goodey, C. J. Mellor, *et al.*, Nano Letters **18**, 498 (2018).

Figures

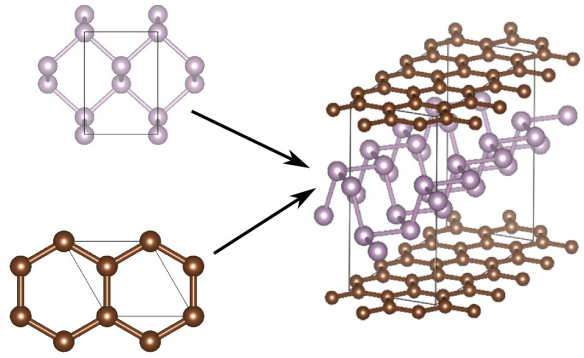

Figure 1: Graphene and phosphorene lattices are stacked on top of each other in order to built the corresponding vdW-heterostructures.

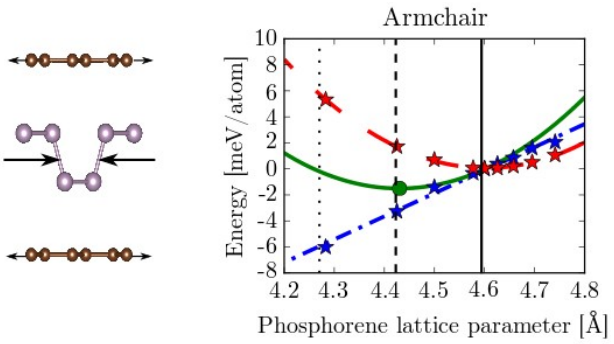

Figure 2: Variation of the intralayer (red), interlayer (blue) and total energy (green) as function of the phosphorene lattice parameter, for different graphene-phosphorene commensurate structures. A contraction of phosphorene armchair lattice parameter is predicted theoretically.