The structure and properties of bilayer borophene

Subrata Rakshit and Nevill Gonzalez Szwacki

Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland

Borophene is a crystalline atomic monolayer of boron that exhibits several polymorphic forms [1]. In recent years, borophene has been identified as a rising star in materials science for the development of sensors, energy storage devices, and batteries.

Very recently it was experimentally demonstrated [2] the synthesis of an atomically well-defined borophene polymorph beyond the single-atomic-layer limit. The structure of the bilayer borophene is consistent with two covalently bonded α-sheets. While these sheets retained the highly desirable electrical and mechanical properties of single-layer borophene, it is proposed that the space between the layers could be used for energy or chemical storage. For example, the inclusion of a layer of lithium ions could enable the manufacture of 2D batteries.

In this work, we present the results of first-principles calculations for double-layer boron structures consisting of hexagonal, α-sheet, or honeycomb boron layers (see Fig. 1). Different arrangements between the layers have been considered. For the most stable structures, the electronic, elastic, and transport properties are studied. According to our calculations, the high metallic character of borophenes is, in most cases, preserved also for the double-layer structures. Also, the structural stability of the single layers is reinforced by the presence of interlayer bonds.

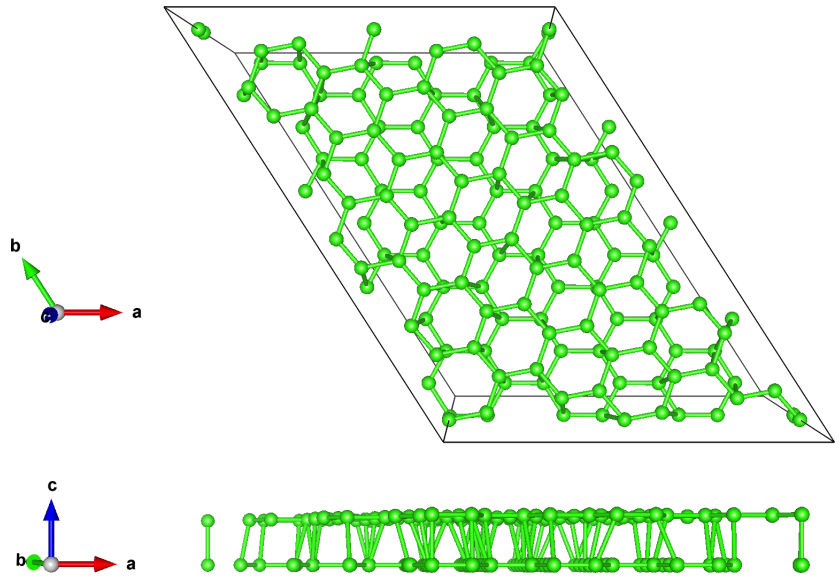

Figure 1: The atomic structure of double layer borophene. The single layers are boron honeycomb (*hc*) structures. The bottom panel shows the bonding between the layers.

[1] T. Tarkowski, N. Gonzalez Szwacki, and M. Marchwiany, *Phys. Rev. B* **104**, 195423 (2021).

[2] X. Liu et al., *Nat. Mater.* **21**, 35 (2022).