Double layer boron structures

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The most stable form of borophene (a one-atom-thick layer of boron), the so-called α-sheet, tends to buckle and therefore is not as stable as graphene and the exfoliation from a substrate may be a challenge [1]. In the bilayer form of 2D boron instead, the interacting layers reinforce each other leading to a more stable structure. Bilayer borophene comprises two atomic-layer-thick sheets bonded together with space between, which could be used for energy or chemical storage. The bilayer material maintains all of α-sheet's desirable electronic properties (e.g. metallic behavior) while offering new advantages. There are theoretical predictions that bilayer borophene is a promising material for batteries (energy storage) since having space between the layers provides a place to hold lithium ions [1].

In this work [2], we present the results of first-principles calculations for bilayer boron structures consisting of two α-sheets. Three distinct arrangements of the layers have been considered: AA, AB, and AB$'$ stackings with $P6/mmm$, $Cmme$, and $P\bar{3}m1$ space groups, respectively. We show that two α-sheets stacked directly on top of each other (AA stacking) form chemical bonds when the distance, d, between planes is 1.8 Å. The boron layers in the AA stacking prefer, however, to be more distant (d = 3.8 Å) which considerably lowers the total energy (see Figh. 1). We have also found that the most stable configuration is the AB stacking in which the boron atoms form an ordered porous tubular structure. According to our calculations, the high metallic character of the α-sheet is also preserved in the double-layer structures.

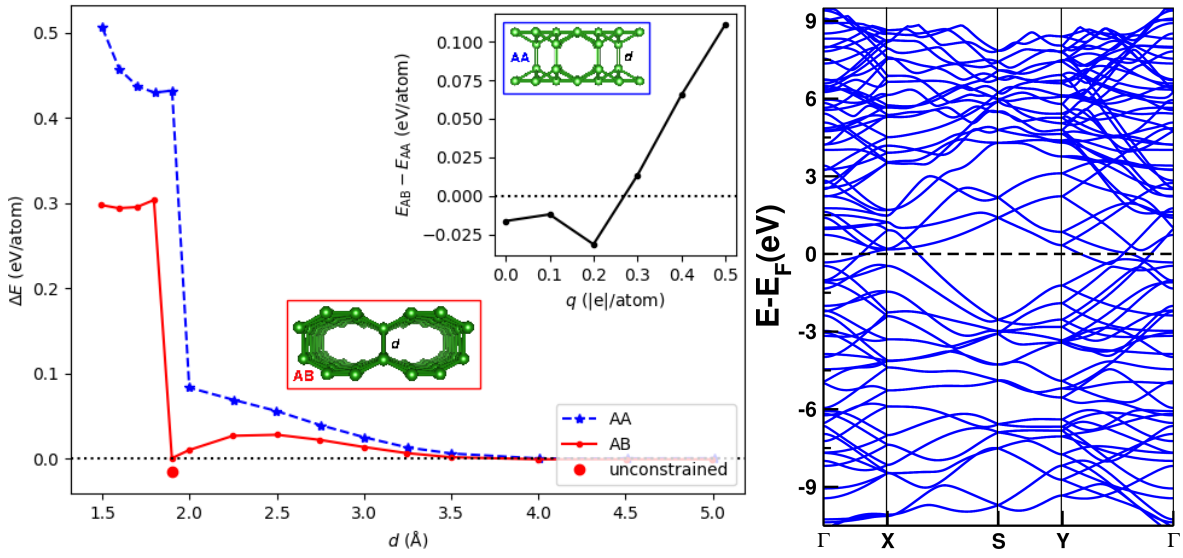

Figure 1: Difference between the energy of the bilayer borophene and the energies of the isolated α-sheets (left). In the inset, it is shown the influence of static charge on the relative stability of AA and AB. The electronic structure of AB (right).

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[1] X. Liu et al., Nature Materials **21**, 35 (2021).

[2] S. Rakshit and N. Gonzalez Szwacki, to be published (2024).