What is the true structure of borophene?

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Two-dimensional systems have emerged as very promising candidates for future electronic devices. Recently, boron joined the distinguished group of elements that are confirmed to possess 2D allotropes, named borophenes [1,2]. However, the structure of the boron sheet strongly depends on the substrate and particular experimental conditions which are employed for its realization. This brings us to a question whether there is a single parameter that predominantly determines the structure of a particular boron sheet. The complexity of the problem may be illustrated vividly by the vast number of different proposals, based on first principles calculations, for the atomic structure of 2D boron crystals – buckled triangular (bt) sheet, one-atom thick layers (α-sheet and related structures [3]), buckled bilayer, bulk-based structures, and other models – that, in principle, could find an experimental realization.

In this work [4], we study the effect of external negative static charge on the stability of boron one-atom thick layers by using a very simple analysis of decomposition of the binding energy of a given boron sheet into contributions coming from atoms that have different coordination number. We express the binding energy of each studied structure as:

$$E_{\mathrm{b}}\left(n_3, n_4, n_5, n_6, q\right) = \frac{1}{N}\sum_{i=3}^{6} n_i e_i^q$$

where n_i and e_i^q are the number of boron atoms in the unit cell with i nearest neighbors (NNs) and their energy, respectively. N is the total number of atoms per unit cell. The individual energy contributions, e_i^q, are found from separate first principles computations for boron sheets in which each atom has i NNs. One example is the graphitic boron structure from which we calculate e_3^q.

By using such a simple model, we established that there is a clear preference in terms of energy for boron sheets with very small or very high (close to $1|e|$) static negative charge per atom. Boron sheets with intermediate charges are energetically not favorable. Our analysis also suggests that under electron rich conditions there should be a clear preference for the formation of the experimentally observed δ-sheet [2], since this structure exhibits the highest binding energy and is composed purely of four- and five-coordinated B atoms, what accounts for the stability. Any static charging seems to be detrimental in terms of binding energy for the bt-sheet, however, this structure undergoes a large 2D volume expansion, what may be helpful in matching to the size of the unit sell of the metallic substrate [1].

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[3] H. Tang and S. Ismail-Beigi, *Phys. Rev. Lett.* **99**, 115501 (2001).
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