Borophene, a polymorphic 2D material

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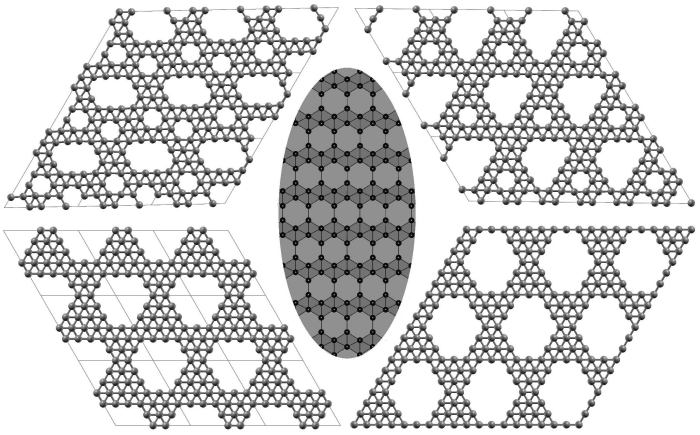
The two-dimensional boron structure in the form synthesized recently [1] was first envisioned theoretically several years ego [2]. Presently, the field of atomically-thin boron, borophene, is evolving rapidly. The vast number of different atomic networks that boron atoms can form – and, what is related, atoms with coordination numbers that vary from 2 to 6 can coexist – makes boron an extremely versatile material in terms of physical and chemical properties and, therefore, potential applications. Despite the huge effort undertaken by researchers to understand the structure and properties of boron allotropes, this element remains one of the less examined not only in its 2D form but also in the molecular, 1D, and bulk forms. The complex and hard work of structure identification could not be nowadays possible without computational modeling [3, 4]. The best example of the synergy between theory and experiment is the largely anticipated [2] and recently obtained [1] boron in its 2D form: δ and γ sheets (the δ sheet is shown in the central part of the figure bellow).

In this work, we make use of cluster expansion and machine-learning techniques to predict the structure of 2D boron allotropes. Some of them are shown in the accompanying figure. The whole range of 2D densities of atoms is considered extending to sparse structures the present knowledge of the structure of 2D boron crystals. We also discuss new possible directions of research in this exciting field and the present and future usage of 2D boron allotropes.



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