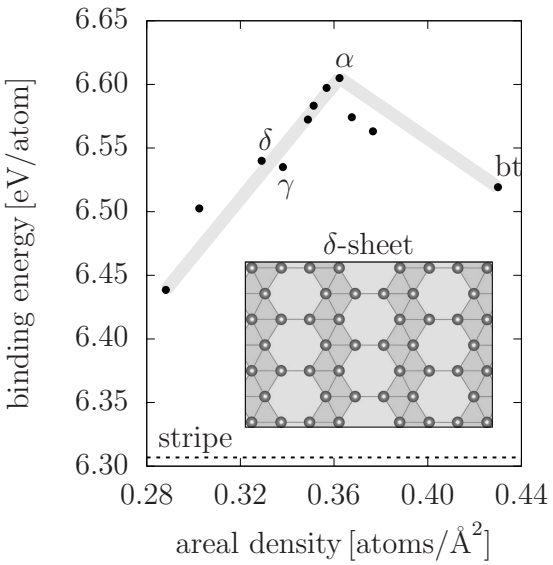
Boron, the most multi-structure material ever

Tomasz Tarkowski, Jacek A. Majewski, and Nevill Gonzalez Szwacki

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

Despite the enormous effort made by experimentalists and theoreticians to understand the structure and properties of boron allotropes, this element remains one of the less examined not only in its bulk form but also in the molecular and 2D forms. 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. The complex work of structure identification could not be nowadays possible without computational modeling. The best example of the synergy between theory and experiment is the largely anticipated by computer simulations (structures e.g. bt – buckled triangular, α, δ, γ sheets, and the stripe, see Figure bellow) and just recently obtained boron in its 2D form (δ and γ sheets) [1, 2].

Here we make a concise but complete review of the present understanding about the different forms that boron can adopt. We start with bulk boron and its 6 confirmed structures, out of about 20 reported, all of them made up from different arrangements of B_{12} icosahedral units directly connected or through additional atoms. Our review continuous with 2D boron that, what should not surprise, can also adopt different structures named borophenes. The story could not be complete without mentioning the molecular allotropes of boron, fullerenes, and its 1D forms like nanowires and nanotubes. The last group of structures is the least understood and seems to be the largest challenge for researchers. Finally, we also discuss new possible directions of research in this exciting field and the present and future usage of the boron allotropes.



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[1] B. Feng *et al.*, *Nature* **8**, 563 (2016).
[2] T. Tarkowski, J. A. Majewski, N. Gonzalez Szwacki, *FlatChem* **7**, 42 (2018).