Borophene, a new wonder 2D material

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Crystal structure prediction is a field of materials science that involves computational science techniques combined with density functional theory to tackle the complex problem of finding the most favorable forms of condensed matter. Borophene, a 2D form of boron, is an example of a material that was completely anticipated theoretically ahead of performing the experiment [1]. Moreover, borophene is a polymorph, a material that can have more than one crystal structure. Since its experimental realization, tremendous efforts have been invested in exploring its synthesis methods as well as in exploiting the potential applications.

Here, we present results of the recent theoretical studies of non-typical forms of borophenes with 2D densities of atoms smaller than those explored so far for 2D boron crystals. Boron atoms in the porous borophenes tend to be 5-coordinated in contrast to commonly investigated structures with mixed triangular and hexagonal motifs for which the number of nearest neighbors of each atom varies from 3 to 6. High metallic character is the usual property of borophenes, however, we have also identified a semimetallic borophene that turns into semiconductor upon unit cell expansion. This extends the possible applications of borophenes to semiconductor industry.

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[1] N. Gonzalez Szwacki and I. Matsuda, "*A historical review of theoretical boron allotropes in various dimensions*", in *2D Boron: Boraphene, Borophene, Boronene*, edited by I. Matsuda and K. Wu (Springer Nature, Switzerland, 2021).