Electronic struture of novel 2D MAB phases

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The two-dimensional (2D) nanostructures have received much attention due to their wide variety of application in different field. The 2D materials such as the layers of transition metal borides called MBenes are comparatively new [1, 2]. Similarly, like MXenes materials, which have been widely studied so far [3], MBenes can be chemically exfoliated from their bulk counterparts (MAB phases).

In this communication we preset a comprehensive *ab initio* studies of 2D MBenes structures in the framework of the Density Functional Theory (DFT). We examine the orthorhombic and hexagonal structures with various concentration of surface functionalization groups: -OH, -H, -O, -Cl, -H. We discuss the issue of the structural phase transition. We examine both magnetic FeB and nonmagnetic MoB MBenes layers. Our results reveal that the pure systems are metallic, however, for particular concentration and arrangement of the surface groups, the materials turn to exhibit semiconducting behavior. In addition, an impact of the number of the layers on the electronic properties is also considered.

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