Exploring structural, electronic, and magnetic properties of 2D Cr, Fe, and Zr monoborides

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MBenes, a family of two-dimensional transition metal borides, has recently attracted significant attention [1]. Their elemental compositions, surface terminations, geometrical forms, and chemical and physical properties are unique and fascinating. These two-dimensional compounds hold promising applications in various fields such as molecular sensing, Li- and Na-ion batteries, electrocatalysis, and magnetic devices. Also important are their exceptional electrical conductivity, high hydrophilicity, rich surface chemistry, and outstanding stability.

In this work [2], we present the results of density functional theory-based calculations for 2D Fe_2B_2, Cr_2B_2, and Zr_2B_2 hexagonal and orthorhombic MBenes. According to our calculations, the orthorhombic form of the 2D structures is the most energetically favorable for Fe_2B_2 and Cr_2B_2, whereas, Zr_2B_2 MBene prefers to adopt the hexagonal form. From phonon calculations, we can also deduce that the orthorhombic structure of Zr_2B_2 and the hexagonal Fe_2B_2 are also structurally stable. The magnetic properties of the two-dimensional systems were also studied and Fe_2B_2 and Cr_2B_2 are found to be ferromagnetic, whereas Zr_2B_2 is nonmagnetic. The Fe_2B_2 structure exhibits a magnetic moment of 3.73 Bohr magnetons per unit cell (see the DOS picture shown in Fig. 1) followed by Cr_2B_2, with 2.58 Bohr magnetons per unit cell. Transport computations reveal that the highest conductivity may be expected for Zr_2B_2 and the smallest for Fe_2B_2. A detailed comparison with available data in the literature will be provided.

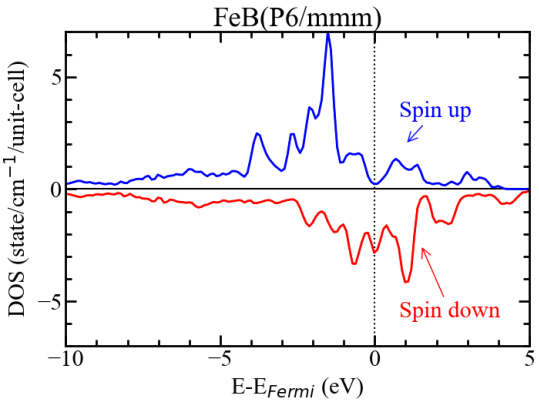

Figure 1: Spin resolved density of states (DOS) of ferromagnetic Fe_2B_2. The upward and downward plots show the majority and minority states, respectively, and the dashed line shows the Fermi energy.

[1] B. Zhang, J. Zhou, and Z. Sun , *J. Mater. Chem. A* **10**, 15865 (2022).
[2] I. Arias Camacho and N. Gonzalez Szwacki, *Materials - Special Issue* (2023).