Band gap engineering of two-dimensional ScB MBene

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MBenes, an emerging member of the two-dimensional (2D) materials, is drawing enormous attention due to their unique mechanical and electronic properties with its diverse crystal symmetries and structures that make them a promising candidate for different types of applications [1, 2]. However, the intrinsic metallic nature of pristine MBenes can be an obstacle for several applications in optics involving photon absorption, emission, and electronics. In a semiconductor material, the band gap is the most crucial parameter, and much effort is put into searching for new nanomaterials with a wide range of band gaps. Although the MBenes exhibit generally metallic behavior, they can be tuned to semiconducting through band engineering. In this work, the electronic band structure of ScB MBenes has been modified utilizing band engineering techniques like surface functionalization and straintronics. We have investigated various crystal symmetries of ScB MBenes and examined their structural and dynamic stability. Our results reveal that ScB with hexagonal crystal symmetry is found to be the most stable one. The electronic structure of ScB with O-, F-, OH- and H-functional groups have been examined and the band structure calculations reveal that the ScB functionalized with O turns out to be semiconducting with a band gap of around 0.1 eV and 0.5 eV within the DFT+U and hybrid exchange correlation functional HSE06, respectively. In addition to functionalization with O, the applied in-plane biaxial strains further enhanced the band gap by 0.8 eV. This can lead the ScBO MBene to take advantage of electronic, optical and several other applications.

References:

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