

Stacking and Strain Controlled Interlayer Coupling and Electronic Transport in Bilayer Borophene

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Abstract

Two-dimensional (2D) boron, commonly termed borophene, has emerged as one of the most structurally diverse elemental 2D materials. Early first-principles studies showed that unlike graphene, stable boron sheets are built from triangular networks with ordered hexagonal holes, stabilized by competing two-center and three-center bonding [1]. In this work, we perform DFT calculations on porous B_{18} -based bilayers [2] in AA and AB stackings, considering for each a covalently bonded minimum and a vdW-separated minimum. We studied their relative stability under biaxial strain and found stacking-dependent, strain-driven switching between bonded and vdW-like structures. Electronic structure analysis shows that the covalent AA bilayer exhibits a Dirac-like feature near the Fermi level dominated by P_x and P_y orbitals. Using a Wannier tight-binding model, we compute the Z_2 invariant and identify a non-trivial phase with gapless edge states, whereas the other stackings remain multiband semimetals without a global gap. Finally, within Boltzmann transport theory, we show that the in-plane conductivity is strongly stacking dependent and is significantly reduced in the vdW-separated bilayers.

References

- [1] H. Tang and S. Ismail-Beigi, Physical Review Letters 99, 115501 (2007).
- [2] T. Tarkowski, N. Gonzalez Szwacki, and M. Marchwiany, Physical Review B 104, 195423 (2021).

Figures

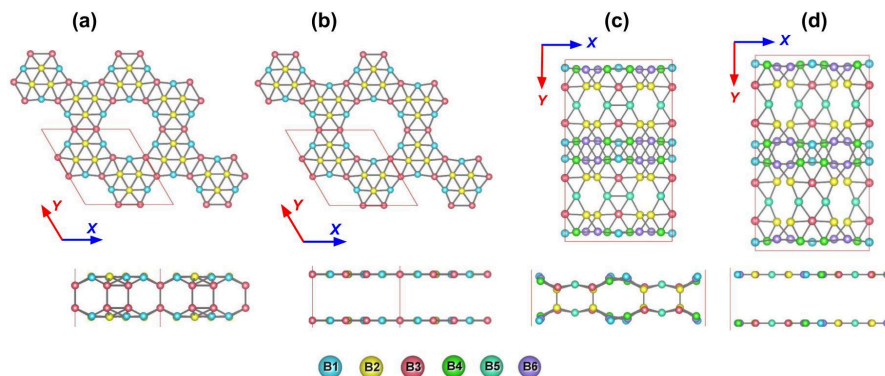


Figure 1: The structures of (a) AA, (b) AA_{vdW} , (c) AB and (d) AB_{vdW} borophene.