Effect of Hydrogen Edge Passivation on BC_3 Ribbons

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Abstract

Interesting electronic properties of graphene has motivated the exploration of other two-dimensional materials. BC_3 is one such material consisting of honeycomb lattice with a homogeneous distribution of boron atoms in sp^2-hibridized network. Unlike graphene, BC_3 exhibits semiconducting behavior arising from Kekule-like charge localization with aromatic carbon hexagons, separated by anti-aromatic hexagons consisting of carbon and boron atoms.

Here we study the quasi one-dimensional ribbon structures of BC_3 with both armchair and zigzag edges mainly highlighting the effect of hydrogen passivation of edge atoms. We observe that, the removal of passivating hydrogen from the edge boron atoms makes them sp-hybridized, increasing their stability by enhanced aromaticity.

The semiconducting armchair ribbons become metallic upon removal of passivating hydrogen from edge borons (see Figure (a)). This metallicity is a consequence of enhanced aromaticity along the edge. With increase in ribbon width, the bulk semiconducting property prevails, giving rise to an anomalous behavior of gap opening (see Figure (a))[1]. In case of semiconducting zigzag ribbons, the removal of passivating hydrogen atoms from edge boron atoms produces robust edge states at Fermi energy and consequent metallicity (see Figure (b)) which does not change upon increase in width[2]. All these observations are confirmed by projected density of states and wave-function analysis.

References

[1] Sudipta Dutta and Katsunori Wakabayashi, J. Mater. Chem. **22** (2012) 20881.
[2] Sudipta Dutta and Katsunori Wakabayashi, J. Mater. Chem. C **1** (2013) 4854.

Figure

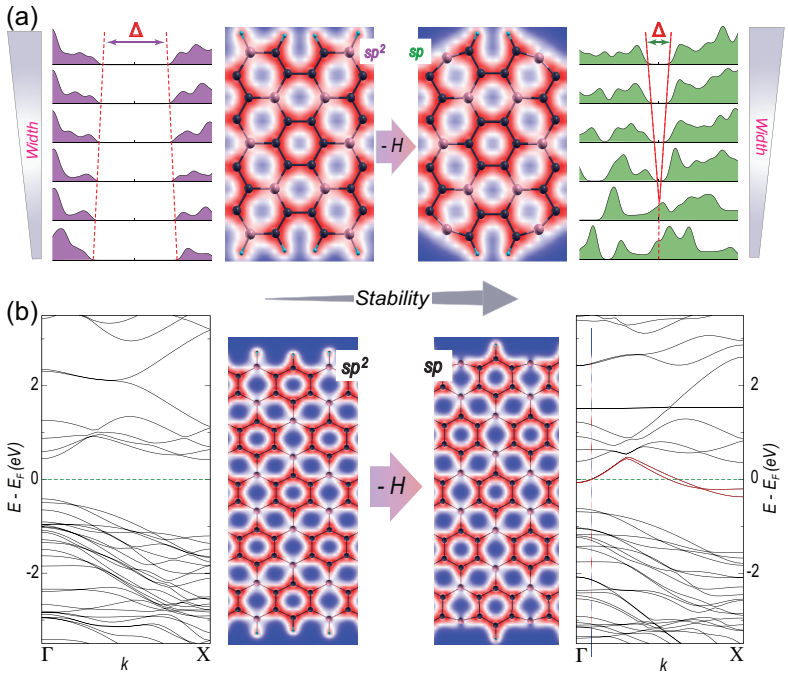

Figure: (a) *The density of states with increase in width of armchair BC_3 ribbons with (left) and without (right) passivating hydrogen atoms on edge boron atoms.* ***(b)*** *The band structures of zigzag BC_3 ribbons with (left) and without (right) passivating hydrogen atoms on edge boron.*