Hybrid states at interfaces of zigzag Graphene/BN heterostructures

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Abstract

It is well known that in zigzag graphene nanoribbons (ZGNRs), the top of the valence band and the bottom of the conduction band are always degenerate at $k = \pm\pi/a$, forming states localized in the vicinity of the zigzag edges. These edge states appear in the band structure as nearly flat bands, i.e. with nearly zero group velocity (Fig. 1), i.e. they cannot contribute significantly to the conduction [1,2]. Recently, studies of topological insulators (TIs) have revealed the existence of states with very high group velocity localized at the surface or edge of samples, while bulk states have the usual properties of states in conventional insulators [3]. Taking advantage of the fact that it is now possible to grow in-plane heterostructures of hexagonal BN (h-BN) and graphene on the same monolayer [4], by means of atomistic simulation we have evidenced the emergence of interface states that look like edge states in ZGNRs but with high group velocity, as can be observed in TIs (Fig. 2). These interface states are localized in the graphene side of G/BN structures. Their maximum group velocity reaches 4.3×10^5 m/s at B-C interfaces and even 7.4×10^5 m/s at N-C interfaces. Additionally, in the case of asymmetric structure BN/Graphene/BN (with both B-C and N-C interfaces), a bandgap of 207 meV has been shown to be open for BN and graphene sub-ribbon widths of 5 nm. These specific properties suggest new ways to engineer and control the transport properties of graphene nanostructures.

References

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Figures

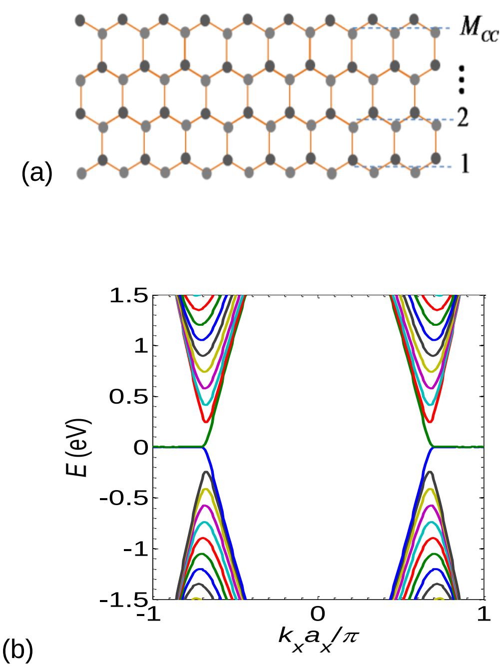

Fig. 1. (a) Pure zigzag graphene ribbon (b) band structure of zigzag graphene for M_{CC} = 50, the flat bands are edge states.

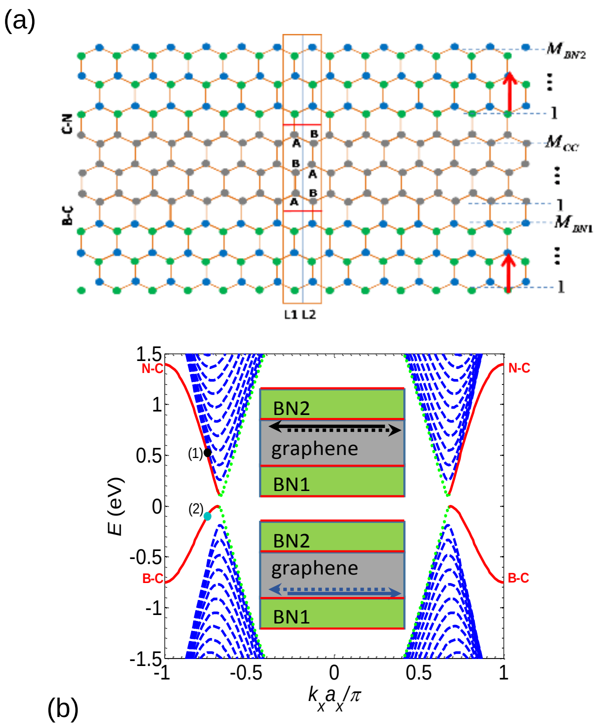

Fig. 2. (a) zigzag BN/G/BN heterostructure with B-C-C-N interface bondings. (b) band structure of B-C-C-N for M_{BN1} = M_{CC} = M_{BN2} = 50 with bandgap and high group velocity hybrid states (red color).