Carrier dimensionality control of multilayer in-plane heterostructure of BN-C

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Graphene can form in-plane heterostructure with hexagonal BN (hBN) owing to their similar ionic radii. These in-plane heterostructures possess unique electronic properties those strongly depend on the domain structures and their arrangement of graphene and hBN [1]. Heterostructures consisting of triangular graphene flakes embedded in hBN have flat dispersion bands, even though sp^2 C atoms form two-dimensional C-C covalent networks [2]. Because of their two-dimensional honeycomb covalent networks, the in-plane heterostructures can form layered structure where the interlayer interaction causes further variation in their electronic properties. Therefore, in this work, we aim to investigate the electronic properties of two-dimensional superlattice consisting of polyacene framework and zigzag hBN ribbons with width of 10 BN chain and its multilayer structure using the density functional theory with generalized gradient approximation (Fig. 1).

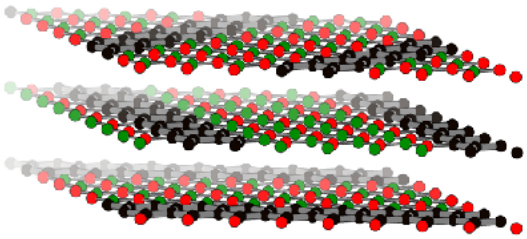

Fig. 1. Geometric structure of multilayer in-plane heterostructure comprising polyacene framework and hBN zigzag ribbons. Black, red, and green balls denote C, B, and N atoms, respectively.

The in-plane heterostructure is a semiconductor with flat dispersion band in its valence band and conduction band edges owing to the border localized states between BC and NC zigzag borders, respectively. By forming trilayer structures, carrier distributions of the band edges of trilayer BNC sheets are sensitive to their stacking arrangement in hBN region. Trilayer BNC structures with AA', AB (B-N-B stacking), AB (N-B-N stacking), and ABC stacking arrangements have 2D, 1D, 2D, and 1D carriers, respectively, in their valence band edges (Fig. 2). These stacking dependent carrier distribution is ascribed to the modulation of the electrostatic potential due to the formation of the multilayer heterostructures.

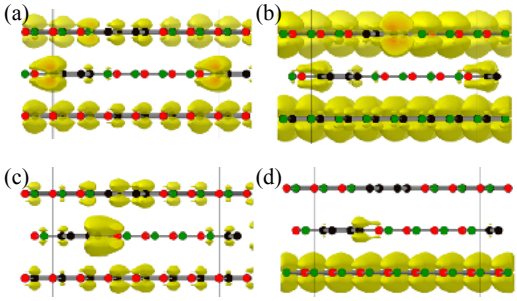

Fig. 2. Carrier distribution in the trilayer BNC structures with (a) AA', (b) AB(B-N-B stacking), (c) AB (N-B-N stacking), and (d) ABC stacking at the highest occupied state at the Γ point.

References

[1] S. Okada et al. Phys. Rev. B **62**, 9896 (2000).
[2] H. Zhang et al. submitted to Jpn. J. Appl. Phys.