Structural, electronic and transport properties of quasi-1D BNC heterostructures.

Simon M.-M. Dubois, Xavier Declerck, Jean-Christophe Charlier, Mike C. Payne

Cavendish Laboratory, University of Cambridge,
19, J J Thomson Avenue, Cambridge CB3 0HE, United Kingdom
smmfnd2@cam.ac.uk

Two dimensional hexagonal BN (*h*-BN), an isomorph of graphene with a lattice mismatch of only 1.7%, is a wide gap insulator as its bulk counterpart [1]. Advances in the synthesis of hybrid BNC heterostructures offer new opportunities to engineer the electronic properties of low-dimensional systems. Recently, it has been shown that the introduction of *h*-BN nanodomains into graphene enables to induce a tunable band gap in the honeycomb lattice [2]. Besides, lateral junctions between electrically conductive graphene and insulating *h*-BN provide new ways to embed electrically isolated elements within single atomic layers [3].

Not only the two-dimensional BNC heterostructures hold promises for new applications but also the corresponding quasi-1D nanoribbons. In this work, we detail the impact of the edges on the stability and electronic structures of graphene and *h*-BN nanoribbons and we explore the electronic and transport properties of various prototypical quasi-1D BNC systems. Our results, obtained by means of first-principles calculations, emphasize the potential of those systems for applications in future electronic and spintronic devices.

References

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