Hybrid states and bandgap in zigzag Graphene/BN heterostructures

V. T. Tran, J. Saint-Martin, and P. Dollfus
IEF, Université Paris-sud, CNRS, UMR 8622, Bât 220, 91405 Orsay, France
e-mail: philippe.dollfus@u-psud.fr and van-truong.tran@u-psud.fr

INTRODUCTION

It is well known that in the band structure of zigzag graphene nanoribbons (ZGNRs) edge states appear as nearly flat bands, i.e. with nearly zero group velocity (Fig. 1c), and thus they cannot contribute significantly to electron transport.[1] However, studies of topological insulators (TIs) have revealed the existence of states with very high group velocity localized at the surface or edge of samples.[2] 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,[3] 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 it can be observed in TIs.

MODEL

Zigzag Graphene/BN heterostructures with different configurations of interfaces have been investigated. The notation "B-C" ("N-C") refers to interfaces where only Boron (Nitrogen) atoms are bonded with Carbon atoms. Fig. 1b shows a "one-interface" system with B-C interface, while a "two-interface" system, noted as B-C--C-N, is schematized in Fig. 3. Hamiltonians were developed within a Tight Binding (TB) model up to second neighbor interactions. Parameters were taken from [4]. The properties of interface states were investigated in terms of localization of wave functions, group velocity and bandgap.

ONE INTERFACE STRUCTURE

Fig 2a shows the energy bands of the B-C structure. It is clear that the flat bands in the first valence band of pure graphene ribbon in Fig.1c are now replaced by downward bended bands (red lines) localized at the interface of Graphene/BN (Fig 2b). These states with high velocity are specific of the B-C interface. We name them "hybrid states".

TWO INTERFACE STRUCTURE

Hybrid states at N-C interface have been also studied. Fig. 3 shows a structure with two BN regions attached to a graphene ribbon forming both B-C and N-C interfaces. Band structure and wave functions are analyzed in Fig 4. The flat bands previously evidenced in B-C structure are no longer present in this B-C--C-N system. New upward bended curves with states localized at the N-C interface emerge. They are hybrid states specific of the N-C interface.

HYBRID STATES: SPECIFIC PROPERTIES

A comparison of group velocities in different structures is shown in Fig 5a. The 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. At given energy, hybrid states in B--C-C-B, N-C--C-N (not shown) propagate at both interfaces as the ones in TIs, while transport interface can be selected in B-C--C-N structure as a function of energy. Additionally, a bandgap of 207 meV can be open in B-C--C-N structure in the case of sub-ribbon widths of 5 nm (Fig 5b).

The role of B(N) atoms in the formation of hybrid states can be intuitively understood by applying on each side of a pure zigzag graphene ribbon two different effective potentials, as sketched in Fig 6a. These potentials are equal to 1.394 eV and -0.75 eV, respectively, i.e. the actual energy values of the hybrid states at the Brillouin zone edge in Fig. 4(a). This approach makes it possible to mimic the dispersion and hybrid edge states in graphene/BN heterostructures, as shown in Fig 6c.

ISBN 978-0-692-50554-0

CONCLUSION

We have evidenced the emergence of dispersive edge states at the interfaces of zigzag graphene/BN in-plane heterostructures. Their specific properties suggest new ways to engineer and control the bandgap and carrier transport properties in graphene nanostructures.

REFERENCES

[1] A. Cresti, G. Grosso, and G. Parravicini, *Electronic states and magnetotransport in unipolar and bipolar graphene ribbons*, Phys. Rev. B **77**, 115408 (2008).

[2] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, *Quantum spin Hall effect and topological phase transition in HgTe quantum wells*, Science **314**, 1757 (2006).

[3] Y. Gao, Y. Zhang, P. Chen, Y. Li, M. Liu, T. Gao, D. Ma, Y. Chen, Z. Cheng, X. Qiu, W. Duan, and Z. Liu, *Toward Single-Layer Uniform Hexagonal Boron Nitride-Graphene Patchworks with Zigzag Linking Edges*, Nano Lett. **13**, 10 (2013).

[4] G. Seol and J. Guo, *Bandgap opening in boron nitride confined armchair graphene nanoribbon*, Appl. Phys. Lett. **98**, 143107 (2011).

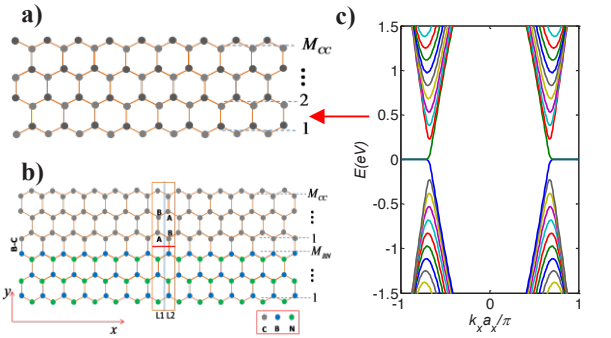

Fig. 1. a) A pure zigzag graphene ribbon. b) Zigzag graphene/BN with B-C interface. c) Band structure of zigzag graphene ribbon for M_{CC} = 50 chain lines.

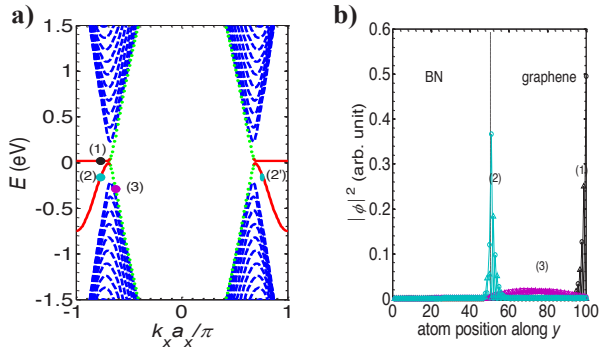

Fig. 2. a) Band structure of B-C structure for $M_{CC} = M_{BN} = 50$ chain lines. b) Wave function of states (1), (2) and (3).

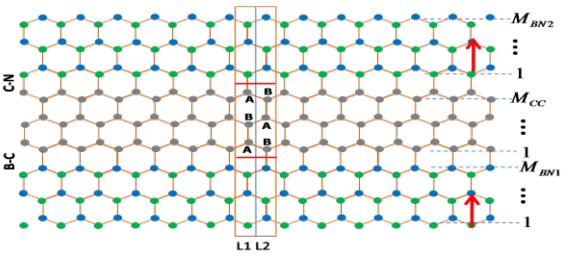

Fig. 3. Graphene/BN zigzag heterostructure with 2 interfaces.

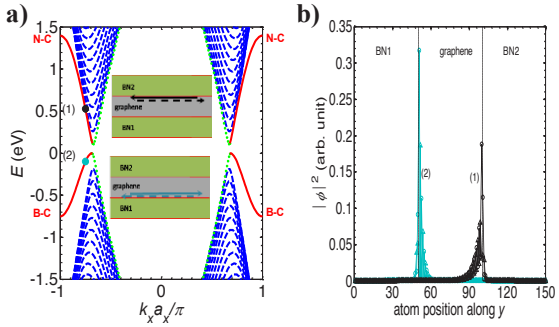

Fig. 4. a) Band structure and b) Wave functions in B-C--C-N heterostructure.

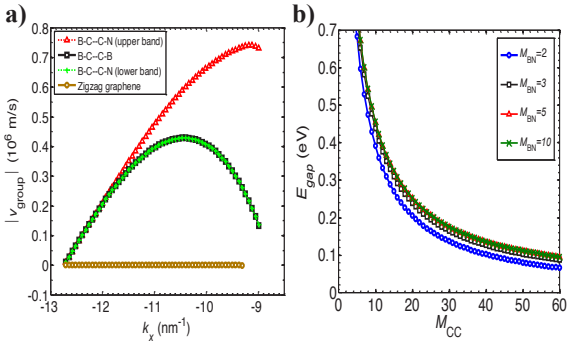

Fig. 5. a) Group velocity in different structures. b) Bandgap in B-C--C-N structures as a function of the graphene width.

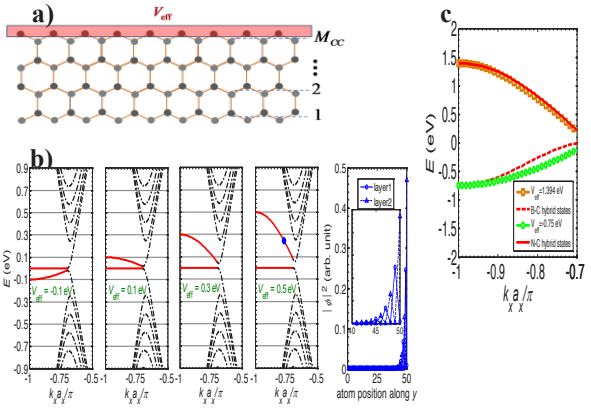

Fig. 6. a) & b) Effective model with a potential V_{eff} applied only on edge atoms of ZGNR. c) Comparison of dispersion of edge states in the effective model with actual dispersions.