

AB INITIO STUDY OF GRAPHENE/BN VAN DER WAALS HETEROSTRUCTURE: EFFECT OF ELECTRIC FIELD, TWIST ANGLES AND P-N DOPING ON THE ELECTRONIC PROPERTIES

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One of the most important and attractive property of 2D materials is the possibility to design brand-new structures, without a bulk counterpart, with innovative features. These systems, known as Van der Waals heterostructures, are characterized by strong covalent bonds between atoms in the same plane and weak Van der Waals interaction among the layers. The key point in the design of new Van der Waals heterostructures lies in the possibility of finely tuning the optoelectronic properties of the system by changing structural parameters[1, 2] like stacking sequences, number of layers and different rotation angles. This aspect is one of the most widely used approaches in the study of novel graphene-based nanodevices. The aim of this work is to study, via DFT calculations, performed with the Quantum ESPRESSO suite, Van der Waals heterostructures based on graphene and hexagonal boron nitride (hBN), two systems with a very similar crystal structure (they have almost the same lattice parameter), but with totally different electronic properties. The goal is to explore different ways to modify the electronic properties of graphene, altering the dispersion of its band structures near the K point of the first Brillouin zone. Starting from the monolayers, several VdW-hs have been designed changing both the number of layers and their relative rotation angle in the structure. In particular, the attention has been focused on the bilayer phase (CBN-AB), the quadrilayer (CBNBNC), and the coincidence lattice achieved by rotating graphene on hBN by 21.8°. For all these systems stability analysis, structural relaxation, band structure calculation and optical properties study have been performed. The intention is to investigate the changes induced by both the structural design itself and by the external environment, investigating the response to an external electric field. The calculations show a small but significant modification [3] of the electronic properties of graphene and hBN when they are paired in a Van der Waals heterostructures, that results in particular in the opening of a tunable [4] band gap at the Dirac cone of graphene, even if the electronic fingerprint of the starting monolayers is still preserved. The results depict the interaction between the C atoms in graphene layers and the B (or N, according to the stacking sequence) atoms in the BN layer as the main factor affecting the electronic behaviour near the Dirac cones. A proper choice of the stacking sequence can induce in the heterostructure a small intrinsic dipole that can further affect the dispersion of the band structure contributing to the opening of small and finely tunable band gap in the Dirac cones of graphene. This makes graphene/hBN hs exploitable for nanoelectronic applications like in THz devices.

References

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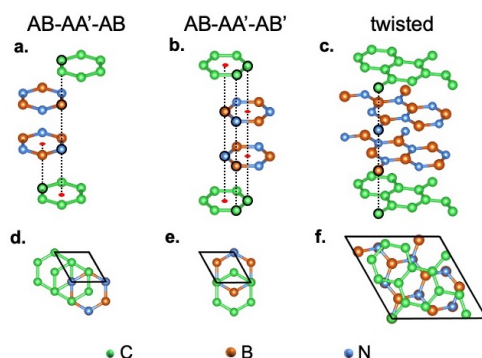


Figure 1: Geometry

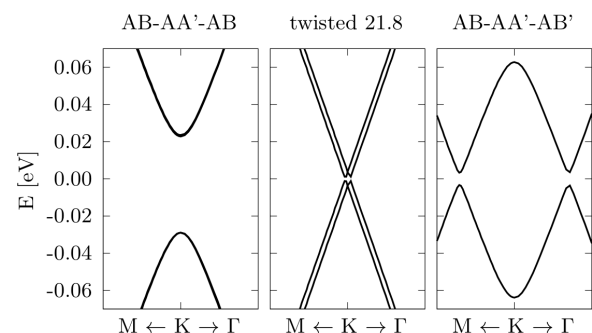


Figure 2: Bands

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