

## Theoretical study of electronic properties of graphene on a BN monolayer substrate

Rafael Martínez-Gordillo<sup>1</sup>, Frank Ortmann<sup>2</sup>, Stephan Roche<sup>2</sup>, Miguel Pruneda<sup>1</sup>

<sup>1</sup>Centre d'Investigació en Nanociència i Nanotecnologia,  
CIN2. (CSIC-ICN), 08193 Bellaterra, Barcelona, Spain

<sup>2</sup>CIN2 (ICN-CSIC) and Universitat Autònoma de Barcelona,  
Catalan Institute of Nanotechnology, Campus UAB, 08193, Bellaterra, Spain  
[rmartinez@cin2.es](mailto:rmartinez@cin2.es)

### Abstract

To take advantage of the electronic properties of graphene in new technology, it is important to consider the effect of the substrate over which graphene is grown as this has an important impact in the structure, symmetry, appearance of charge impurities and doping effect [1,2,3]. Boron nitride (BN) is an insulator that offers improved properties as a substrate for graphene, keeping the intrinsic properties like the high mobility [4] and semimetallicity [5] to an acceptable degree, also avoiding ripples and charge inhomogeneities [6]. Even though, the coupling between boron nitride layer and graphene is weak, the variations in the potential felt by graphene due to the underlying BN have important consequences. The slightly mismatch in lattice parameter and the rotation angle formed by the two lattices give rise to moiré patterns (Figure 1) that have been experimentally observed. The weak modulated potential of the underlying BN-sheet creates new Dirac points at energies above and below the Fermi level [7], having an important impact in the density of states, and thus, giving place to new physics not yet well understood.

In this work, the effect of BN monolayer used as a substrate for graphene is analyzed by means of first-principles calculations using DFT as implemented in the SIESTA package [8]. We considered three rotation angles between BN and graphene lattices using three different supercell sizes. For all the studied systems the calculated DOS show dips at the positions of the new Dirac cones as reported experimentally in Ref. [7]. The position of these dips depends on the periodicity of the moirés  $\lambda$ , getting closer to the Fermi level as the  $\lambda$  increases, although the energy of these Dirac points do not fully agree with the perturbative expression given in Ref. [7]. Also, the depth of these features increases as the periodicity of the potential increases. Although a depletion is found, the depth is smaller than what is seen by STM or by modeling the system with tight-binding (TB) parameters [7]. We suggest that one possible explanation for this is that the STM tip applies pressure on the sample decreasing the interlayer distance.

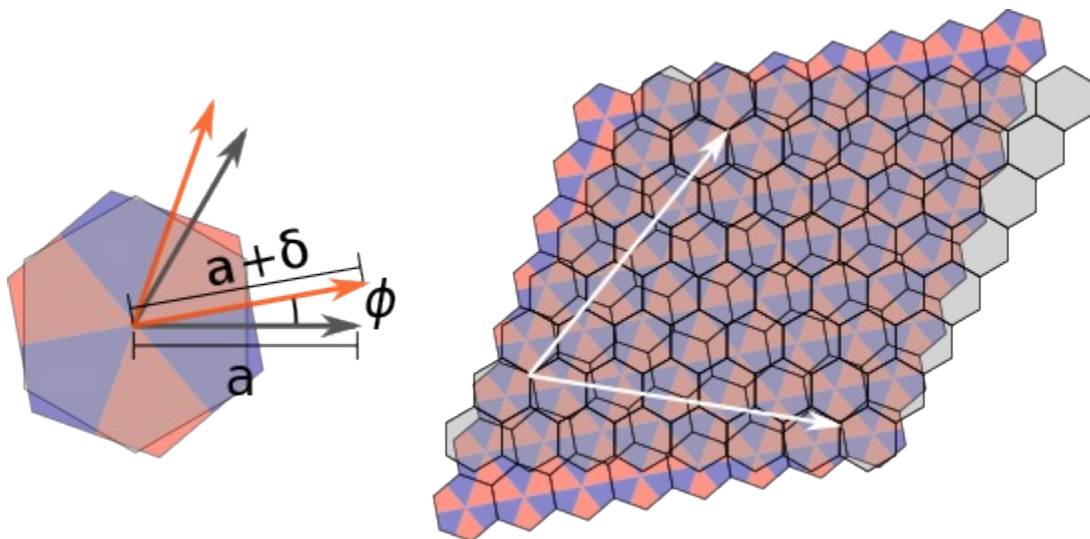
We compared our results to the TB model proposed by Sachs *et al.* [9] that describes the behavior of the biggest cell of the moiré pattern (with a rotation angle between both lattices of 0°). This model considers only graphene, with a modulation term in the on-site energy, so that the BN part is not explicitly treated in the hamiltonian. This term describes the change in the potential felt by graphene due to BN lowering and rising depending on the local conformation of the moiré pattern. By considering this

TB model, we can simulate larger systems to explore the effect of disorder on the moiré potential and the impact on mesoscopic transport. To represent impurities and structural dislocations we used Anderson disorder, that is added as a random uncorrelated change in the on-site energy. We show that the underlying moiré pattern has important consequences on the electronic properties.

## References

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## Figures



**Figure 1.** Construction of the moiré pattern with graphene lattice parameter  $a$  and BN lattice parameter  $a+\delta$ . The rotation angle  $\phi$  determines the size of the supercell.