Moiré-induced Dirac cones replicas and minigaps opening in graphene/hBN superlattices

Simone Brozzesi[1], Alberto Zobelli[2], Maurizia Palummo[1], Olivia Pulci[1]

[1]Department of Physics, University of Rome Tor Vergata, Rome, Italy

[2]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, Orsay, France

Corresponding author: olivia.pulci@roma2.infn.it

Moiré pattern is a novel and extensive structure that emerges from the interference of multiple periodic templates. In condensed-matter physics, moiré patterns, also known as moiré superlattices, can be created by stacking two or more two-dimensional (2D) layered materials with a small twist angle and/or a slight lattice mismatch. The presence of moiré pattern results in the formation of a long range moiré potential, which interacts with the electrons of the system and affects the dispersion of the energy levels. In recent years, moiré superlattices have garnered significant attention due to their remarkable manifestation of previously unexplored phenomena and unique functionalities [1], like strongly correlated phases [2] and subsequent observation of superconductivity and topological states [3], and exotic excitonic states [4] arising from the interaction between excitons and moiré potential. The aim of this study is to demonstrate that the existence of a moiré pattern in a graphene/hBN heterostructure has a substantial influence on the energy levels dispersion of the system. In particular, there is the intention to show that this influence goes beyond the coupling between the planes and the rehybridization of levels that can be expected in van der Waals heterostructures, but significantly affects the energy levels dispersion of graphene within an energy range inside the hBN gap, where only contributions from C atoms are expected to be present. By means of DFT calculation based on a localized basis set approach, this study demonstrates that the presence of the long range moiré potential results in the formation of six replicas [5] of the graphene Dirac cones around the K-K' point of the 1BZ of graphene, which are separated by a reciprocal space superlattice vector G_m from the main cone. The intersection between the main cone and its replicas result in the opening of minigaps in the energy levels of graphene, without the direct interplay of the interaction with the hBN states. The relative positions of these minigaps is dependent on the moiré reconstruction of the system and can be tailored by tuning the rotation angle between the layers.

[1] Lifu Zhang, Ruihao Ni, and You Zhou, Journal of Applied Physics 133.8 (2023)

[2] Yuan Cao et al., Nature 556.7699 (2018), pp. 80–84

[3] Yuan Cao et al., Nature 556.7699 (2018), pp. 43–50

[4] Yuan Cao et al., Science advances 3.11 (2017), e1701696

[5] Ivo Pletikosić et al., Physical review letters 102.5 (2009), p. 0568088