Electronic properties of Twisted Bilayer Graphene with vacancies

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Abstract

Graphene bilayers (BLG), with AA or AB (Bernal) stacking have been known for several years[1]. AA stacking corresponds to a rotational angle of 0° while AB stacking corresponds to an angle of 60°, but in fact, nothing prevents us to build systems with arbitrary angle between 0° and 60°. Indeed it has been observed from experiments that graphene layers can be rotated on some substrates[2-4] with an angle between successive layers that ranges from 0° to 60°. These rotations create moiré patterns that are observed on STM images[2]. These rotated (twisted) bilayer graphene (TBLG) differ both from single layer graphene (SLG) and graphite and their electronic structure is governed by the rotation angle. While a large rotation angle ($\theta \sim 30°$) results in two decoupled graphene layers[5-12] with a linear dispersion near the Dirac points, carriers in a twisted graphene bilayer evolve from Dirac fermions to strongly localized electrons (or holes) when the rotation angle is decreased toward very small angles[6] (or increased toward 60°, the system is symmetric with respect to $\theta = 30°$, Fig. 1).

At the intersection between two Dirac cones originating from two different layers, the interaction between the states can open a gap and saddle points appear (Fig. 2). At 2D such saddle points give rise to van Hove singularities (named E_+ and E_- in Fig. 2) characterized by sharp peaks in the density of states (DOS). As θ is brought closer to 0°, the two van Hove singularities fall closer to the Dirac point and eventually merge for θ close to 2°. The van Hove singularities have been recently observed in different systems[4, 13] confirming these theoretical predictions. When the two van Hove singularities merge, the DOS shows a sharp peak at the Dirac point (fig. 2b). States belonging to this peak are localized in the AA region of the moiré pattern[6].

We want to test the robustness of such systems when confronted by the environment. Such environmental factors include doping, strength, defects, vacancies. Here we will focus on vacancies for angles as small as possible permitted by the *ab-initio* DFT simulations. In the small rotational angle limit, the number of atoms scales like $1/\theta^2$ So in order to keep the simulation time reasonably small, we were limited by systems with few hundreds of atoms which give us systems with 508 atoms and $\theta = 5.08°$. We compare how a simple vacancy in different systems (SLG, BLG, TBLG) and different vacancy sites (AA, AB, TOP and HOLLOW) can modify the electronic properties.

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Figures

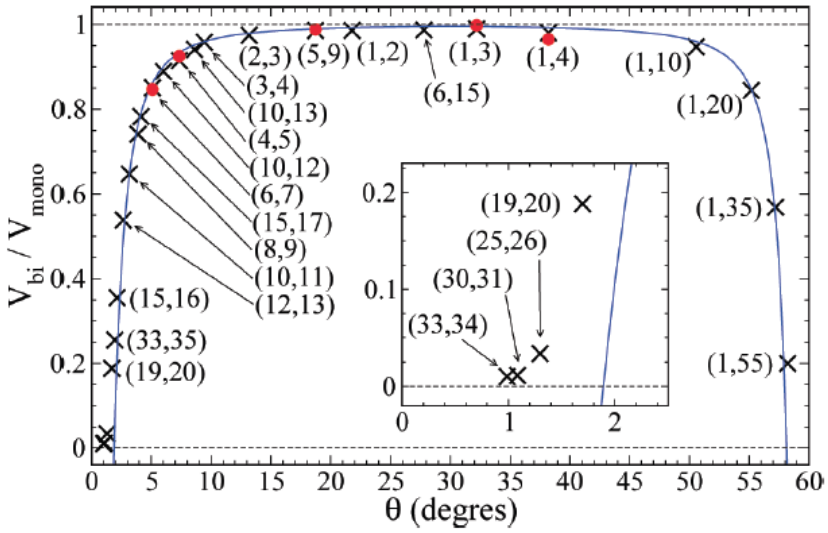

FIGURE 1 – Velocity ratio of bilayer and monolayer graphene for a commensurate bilayer cell versus rotation angle. Circles : DFT calculations ; crosses : TB calculations ; line : theoretical prediction of Lopez dos Santos et al.

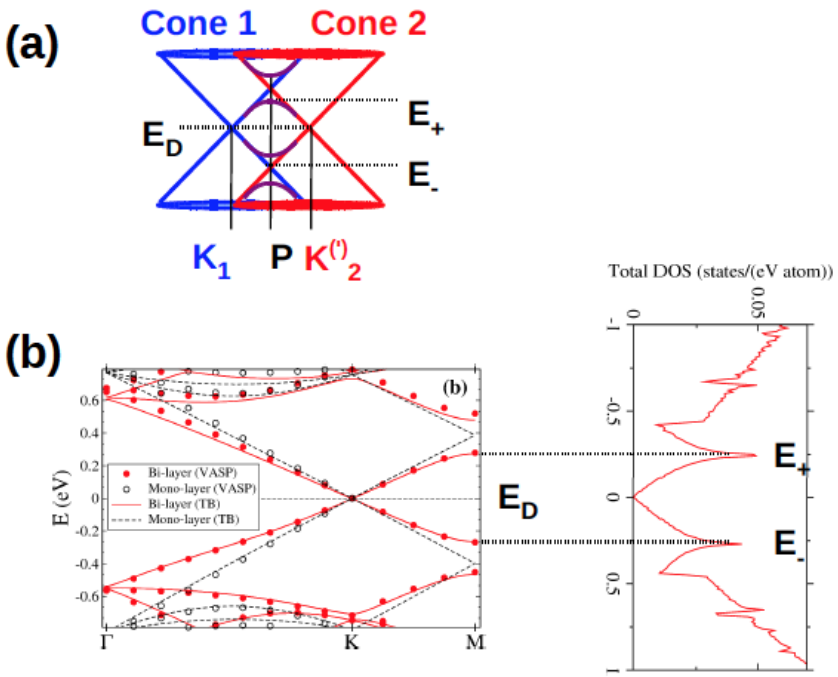

FIGURE 2 – Van Hove singularities of a (6,7) bi- layer. a) schematic drawing, b) (6,7) band structure and total DOS.