On the existence of gapless electronic states in gated bilayer graphene with an array of line defects

Raúl Guerrero  
Marta Pelc  
Andrés Ayuela

Donostia International Physics Center, Centro de Física de Materiales-MPC CSIC-UPV/EHU, San Sebastián-Donostia, Spain.  
rguerrerro@dipc.org

Recent studies on topological insulators, awarded the physics Nobel prize in 2016, boost the current interest of electronic topological states in two-dimensional systems. Bernal stacking bilayer graphene shows a tunable band gap by applying an electric field [1, 2]. Experimental studies on gated bilayer graphene confirm the existence of topological protected gapless states induced by domain walls that change layers stacking from AB to BA [3, 4]. In this work, we investigate bilayer graphene (BLG) with an array of line defects made of pentagons and octagons, allowing to obtain AB/BA stacking changes (see Figure 1). We perform our calculations using first principles calculations including Van der Waals interactions between the layers with an VdW-DF pseudopotential [5, 6]. We firstly test that the energy defect states corresponding to grain boundaries defects are along the Γ-K Brillouin Zone, as reported in previous studies [1, 7]. We then show how the defects equally separated in the perpendicular defect direction. On the other hand, the defects are not aligned one with the other. This cause a change the band structures and topological states near the valley cones K and K’. Last, we shall comment on the role an external electric field between -0.9 to 0.9 (V/Å) perpendicular to the slab, following the protected gapless bands, as mainly proposed for topological protected states in previous tight-binding studies.

References


Figures

Figure 1: Schematic representation of bilayer graphene with AB/BA stacking changes using different ways to align defects within the unit cell. The unit cell is periodic in the direction of the arrows.