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

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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

[1] L. Ju, Z. Shi, N. Nair, et al. Nature, 520 (2015) 650.
[2] B-J. Jiang, G-X. Ni, Z. Addison, et al. Nano Lett. 17 (2017) 7080.
[3] McCann, Phys. Rev. B 74 (2006) 161403.
[4] J. Lahiri, Y. Lin, P. Bozkurt, et al. Nature Nanotech. 5 (2010) 326.
[5] J. Soler, E. Artacho, J. D. Gale, A. Garcia, et al. J. Phys. Condens. Matter 14 (2002) 2745.
[6] K. Lee, E. Murray, L. Kong, B. I. Lundqvist and D.C. Langreth, Phys. Rev. B 82 (2010) 081101.
[7] W. Jaskólski, M. Pelc, L. Chico and A. Ayuela, Nanoscale, 8 (2016) 6079.

Figures

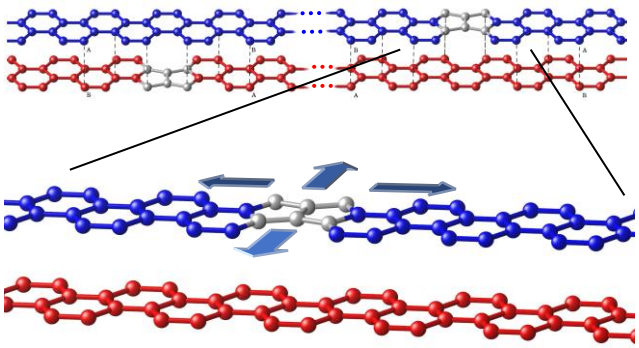

Figure 1: Schematic representation of bilayer graphene with AB/BA stacking changes using different ways to align defects within the unit cell. The unit cell is periodic in the direction of the arrows.