Tarea 1

15 de Octubre

2D materials. By using the tight-binding method, calculate the band structure (or subbands if applies) for the following systems. Always explain what you are doing, what is your Hamiltonian, and what insight you get from your results

1. Graphene monolayer. Addtionally, show analitically, that in the neighborhood of the point K the effective Hamiltonian is the massless 2D Dirac equation.

2. Graphene bilayer in the Bernal stacking. You should reproduce Fig.3 from E. McCann and M. Koshino (2013) Rep. Prog. Phys. **76** 056503

3. Graphene trilayer in the hexagonal staking (AAA). You should reproduce Fig. 1a from Bao *et al.* Nano Lett. (2017) **17** 1564-1568.

4. Make a hexagonally stacked (AAA) graphene trilayer, but changing two C atoms by B^+: one from the top layer, and one from the bottom layer. You don't need to care for any extra electrons. Notice that two arrangement are possible: CB-CC-CB and CB-CC-BC, what is the difference and what are the implications.

5. A graphene nanoribbon along the zig-zag and armchair orientation. You should reproduce Fig. 4 from Peres *et al.* Phys. Rev. B **73**, 195411 (2006)

6. Repeat the nanoribbon exercise, but for the trilayer of 3.

7. Repeat the nanoribbon exercise, but for the trilayer of 4.