Electronic property of the emergent Moiré pattern on single-sided fluorinated graphene studied by tight-binding approach

Renan da Paixão Maciel[1]
Kristofer Björnson, Chin Shen Ong[1], Yaroslav Kvashnin[1], Danny Thonig[2], Olle Eriksson[1 2]

[1] *Uppsala University, Department of Physics and Astronomy, Lägerhyddsvägen 1, 752 37, Uppsala, Sweden*
[2] *Örebro University, Department of Physics and Astronomy, Fakultetsgatan 1, 702 81, Örebro, Sweden*
renan.maciel@physics.uu.se

Graphene has been receiving significant attention since its discovery because of its wide range of applications (e.g. sensors, flexible and high-speed devices, spintronics). The main role of its wide applicability relies on the linear dispersion defined by the Dirac cone at the Fermi level [1], which allows mass-less electrons to be easily conducted from two different terminals. However, there are many interesting ways to manipulate this property in order to understand how graphene electrical attributes are influenced, such as carrier concentration and transport mechanisms. In this sense, one can also induce new features on the graphene band, like creating a gap opening to provide a suitable control of its electrical properties [2]. One way of doing it is by modifying the graphene lattice structure or its bindings through the process called functionalization [2]. Recent work [3] has shown that functionalizing one single side of bilayer graphene with fluorine atoms can induce Moiré patterns phenomenon in the structure, which make it possible to engineer graphene electronic properties with a large supercell structure. Motivated by that, we first study the band structure of the functionalized monolayer graphene in two possible different configurations, namely, C2F boat and C2F chair, via first-principles calculations. Since Moiré patterns are not suitable for DFT calculations because of typically thousands of atoms in the unit cell, we use the tight-binding approach to investigate its electronic structure. By using both approaches, we aim to inspect the influence of the fluorine and of the emergent Moiré pattern on the electronic structure, especially the Dirac cone, and the conductivity of the bilayer graphene.

References

[1] Neto, AH Castro, et al. "The electronic properties of graphene." Review of Modern Physics 81.1 (2009): 109
[2] Sreeprasad, T. S., and Vikas Berry. "How do the electrical properties of graphene change with its functionalization?." Small Nano-Micro (2013): 341-350.
[3] Li, Hu, et al. "Direct writing of lateral fluorographene nanopatterns with tunable bandgaps and its application in a new generation of moiré superlattice." Applied Physics Reviews 7.1 (2020): 011403.