# Theory of the Electronic Structure of Grain Boundaries in Graphene

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Graphene is currently one of the most intensively studied materials because it is expected to find applications in novel nano-electronic devices. Graphene presents frequently grain boundaries and defect lines, which occur spontaneously in the process of growth or can be created on demand. Grain boundaries have been measured to affect both the electronic transport and the magnetic properties of graphene and are the subject of ongoing research. This is because they present localized states with energies at or close to the Fermi level. Such states allow also for the decoration of defect lines with adsorbates, opening a route for nanosensor applications. As the electronic and optoelectronic properties of graphene are modified by the localized states at the grain boundaries, the final control of graphene-based devices requires the tailoring and engineering of such defect lines. However, the relation between the geometry of grain boundaries and the induced electronic localized states has not been so far understood.

Here we treat the defect lines as the outcome of matching of two graphene sheets with different edges, which produces localized states. Recently, general rules to predict the existence of edge-localized states and flat bands at the Fermi level in graphene nanoribbons with arbitrary shape of the edges have been given [1]. The localization at defect lines built of octagonal rings has also been understood as a consequence of the zigzag nature of the graphene edges forming the defect lines [2]. Here we bring into contact these ideas about localized states in graphene edges to give a more comprehensive explanation of states appearing in extended defect lines in graphene. We classify the energy spectra of grain boundaries into a few types only, relating them directly to the basic classes of spectra of graphene edges [1]. We have found a simple formula, which based on the topology of grains, allows to obtain the number of interface bands with energies in the gap and close to $E_F$. This provides a new understanding on states localized at grain boundaries, showing that they are derived from the edge states of graphene, and allowing for the prediction of their electronic characteristics without performing numerical calculations. Such knowledge is crucial for the ultimate tailoring of electronic and optoelectronic applications of graphene.

[1] W. Jaskolski, A.Ayuela, M. Pelc, H. Santos, and L. Chico, *Phys. Rev. B.* **83**, 235424 (2011)
[2] M. Pelc, L. Chico, A. Ayuela, and W. Jaskolski, *Phys. Rev. B.* **87**, 165427 (2013).