# Octagonal defect lines in graphene nanoribbons and carbon nanotubes

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Experimental techniques allow nowadays to pattern graphene into nanometer size ribbons with well controlled size and shape of the edges [1]. Graphene ribbons can be connected by introducing topological defects at their interfaces and it concerns also junctions between carbon nanotubes. Such junctions are interesting because they reveal localized states of magnetic nature at Fermi energy. Junctions between carbon nanotubes are usually realized by pentagon/heptagon topological defects, which strongly mix the graphene sublattices and therefore cannot yield localized states at the Fermi energy. Interfaces between graphene ribbons form one-dimensional grain boundaries, where octagons may also happen. It has been recently shown [2] that such grain boundaries can act as one-dimensional metallic wires.

We study several graphene systems containing octagonal defect lines. All the calculations are performed within the π-electron tight binding approximation. The electron interaction effects are taken into account by means of the Hubbard model. We show that contrary to pentagon/heptagon defects, octagonal defects give rise to localized states at Fermi energy even if the graphene sublattices are mixed. We prove that the localization along chains of octagons is a consequence of the zigzag nature of graphene edges forming the defect lines.

First, we study zigzag graphene ribbon containing defect lines made of octagons only. Although such a system is not a pure graphene structure, there is no sublattice mixing in this case. Four flat bands appear at Fermi energy: two of them are localized at zigzag edges of the ribbon and the additional pair is localized at the line of octagonal defects. The inclusion of electron-electron interaction effects reveals that such a system has spontaneous magnetization of 2 Bohr magnetons.

Next, we consider a system in which every second octagon in the defect line is reconstructed into a pair of pentagons. Such system has been very recently studied experimentally [2]. The presence of pentagons mixes locally both sublattices. Consequently, only one flat band at the Fermi level is localized at the octagonal defect lines. Spontaneous magnetization survives, but drops down to 0.6 Bohr magnetons.

We have studied also rolled-up systems, i.e., carbon nanotubes with octagonal defect lines along the tube axis or at junctions between tubes. We have shown that localization at octagons with energies at the Fermi level is robust and present in all the system considered, independently whether the graphene sublattices are mixed or not. It suggests that octagonal defects can indicate reactivity sites in graphene. Finally, we show that the appearance of localized flat bands at the Fermi energy may be explained using the hybridization rules introduced in Ref. [3] for graphene ribbons with arbitrary edges.

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