Electronic, Magnetic and Transport Properties of Graphene Ribbons Terminated by Nanotubes

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By a combination of density functional (DFT) calculations and large-scale tight-binding (TB) simulations of transport properties we study the electronic and magnetic properties of graphene nanoribbons with edges rolled to form nanotubes[1], an edge structure with low formation energy[2]. We show that, besides protecting the edges from contamination and reconstructions, nanotubes at the edges may lead to magnetism and are not detrimental for the electronic mobility despite the row of sp^3 hybridized atoms at the nanoribbon-nanotube junction.

Edges with armchair nanotubes present magnetic moments localized either in the tube or the ribbon and metallic or half-metallic character, depending on the symmetry of the junction (see Figure1). These properties have potential for spin valve and spin filter devices with advantages over other proposed systems.

Edges with zigzag nanotubes are either metallic or semiconducting without affecting the intrinsic mobility of the ribbon. By varying the type and size of the nanotubes and ribbons offers the possibility to tailor the magnetic and transport properties, making these systems very promising for applications.

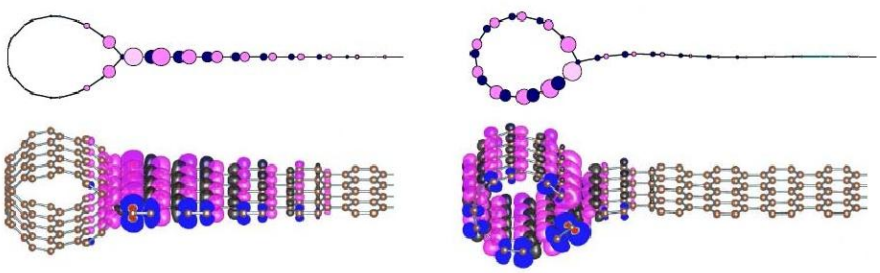

Figure 1: Structure and spin density for symmetric (left) and asymmetric (right) of nanoribbon edges terminated by armchair nanotubes. The localization of magnetization depends on the nanoribbon-nanotube junction.

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