Electronic Structure of Graphene Islands and Ribbons Embedded in Graphene Oxide

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The electronic structure of carbon nanoribbons are, to a great extent, determined by the so-called edge states. For zigzag terminations, these localized states lead to the opening up of a small gap and the stabilization of an anti-ferromagnetic order.

Besides, they allow the spin-dependent modulation of the electronic structure with transverse electric fields leading to a half-metallicity behavior. In this work we investigate the properties of a graphene nanoribbon and nanoislands embedded in graphene oxide layers. These 2D structures may be synthesized by a local anodic oxidation of a graphene layer or local reduction of a graphene oxide layer, employing, for instance, the tip of an atomic force microscopy. The idea is to manipulate the decay characteristic of the edge state and evaluate the effect on the magnetic order and in the electronic structure for the nanoribbons and to analyze the electronic states originated by the graphene islands. We consider several distinct widths for the graphene and graphene oxide layers.

The calculations are based on the Pseudopotential Density Functional Theory as implemented in the SIESTA program. We make use of a basis set composed of pseudo atomic orbitals of finite range and the generalized gradient approximation for the exchange correlation potential. All the geometries are fully optimized.