Edge states in graphene nanostructures on metal surfaces

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Graphene is a fascinating two-dimensional system with unique electronic and transport properties. Nevertheless, the absence of an energy gap in its band structure limits its applicability in semiconductor technology. Fabrication of graphene nanostructures, such as nanoribbons and quantum dots, provides a route to induce the required band gap. Interestingly, zigzag-terminated nanostructures possess electronic states localized at the edge, which lead to non-trivial magnetic properties. In fact, in the case of graphene nanoribbons, mean field calculations predict a ferromagnetic spin polarization along the two edges and an antiferromagnetic coupling across the nanoribbon. These properties have been investigated intensively recently, due to potential applications in the field of spintronics. However, in principle, there exist various effects which can undermine the stability of edge magnetism, including quantum and thermal fluctuations, edge reconstruction and passivation, and, for supported nanostructures, the interaction with the substrate.

In this work, we have focused on substrate effects. For this purpose, we have carried out a density functional theory study of the electronic and magnetic properties of graphene nanoribbons on the (111) surface of several metallic substrates, namely Ir, Au, Ag and Cu. The selected substrates are commonly used to grow graphene nanostructures by chemical vapor deposition methods or bottom-up approaches. We have considered both H-free and H-passivated nanostructures. In the case of the Ir(111) surface, we do not find states localized at the nanoribbon edges. We explain this result by the interplay between a strong and intricate hybridization of the graphene π orbitals with Ir d states and a lattice-mismatch driven geometrical relaxation at the edges. Our simulations are in agreement with scanning tunneling spectroscopy experiments performed on graphene islands on Ir(111). In the case of Au, Ag and Au substrates, the nanoribbons possess edge states. In spite of this, they do not exhibit a significant magnetization at the edge, with the exception of H-terminated nanoribbons on Au(111), whose zero-temperature, mean-field magnetic properties are comparable to those of free-standing nanoribbons. These findings are explained in terms of the different chemical interaction and charge transfer between the nanoribbons and the three substrates.