

Electronic and magnetic properties of graphene nanoribbons deposited on metallic substrates

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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. A route to induce the required band gap is nanostructuring. Recent efforts have focused on one-dimensional graphene nanoribbons and zero-dimensional graphene quantum dots.

According to mean-field calculations, zigzag-terminated nanostructures possess magnetic electronic states localized at the edge. This property has been investigated intensively recently, due to the potential applications in the field of spintronics. However, the robustness of this phenomenon is hotly debated, particularly in the case of supported nanostructures.

In this work, 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 [1], Au, Ag and Cu [2]. Ir and Cu substrates are routinely used for the growth of graphene flakes by chemical vapor deposition. Ag and Au substrates have been successfully employed to fabricate graphene nanoribbons by thermally-induced polymerization of suitable precursor molecules.

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 surprising result by the interplay between a strong and intricate hybridization of the graphene π orbitals with Ir d orbitals and a lattice-mismatch driven geometrical relaxation at the edges. These findings are in agreement with STM experiments performed on graphene islands on Ir(111) [1,3].

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 magnetic properties are comparable to those of free-standing nanoribbons. These results are explained by the different hybridization between the graphene π states and those of the substrates and, for some models, also by the charge transfer between the surface and the nanoribbon [2].

References

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