SAM-like Arrangement of Thiolated Graphene Nanoribbons: Decoupling the Edge State from the Metal Substrate

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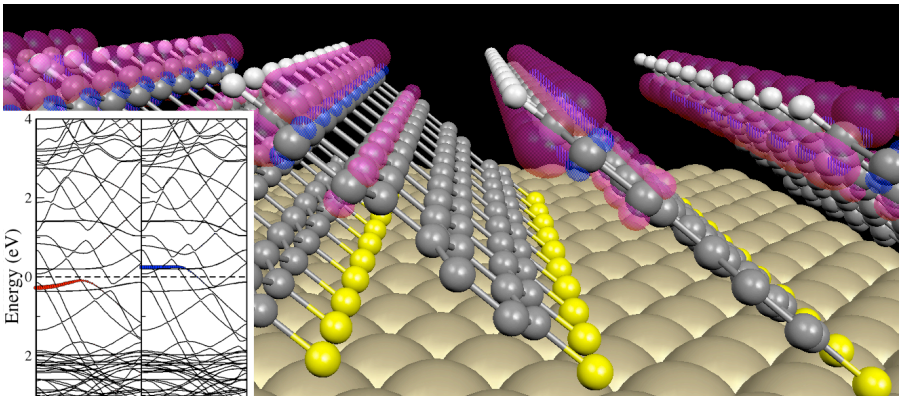
Abstract

Density functional theory calculations have been used to analyze the electronic and magnetic properties of ultrathin zigzag graphene nanoribbons (ZGNR) with different edge saturations. We have compared a symmetric hydrogen saturation of both edges with an asymmetric saturation in which one of the edges is saturated with sulphur atoms or thiol groups, while the other one is kept hydrogen saturated. The adsorption of such partially thiolated ZGNRs on Au(111) has also been explored. We have considered vertical and tilted adsorption configurations of the ribbons, reminiscent of those found for thiolated organic molecules in self-assembled monolayers (SAM) on gold substrates. We have found that saturation with sulphur atoms or thiol groups removes the corresponding edge state from the Fermi energy and kills the accompanying spin polarization. However, this effect is so local that the electronic and magnetic properties of the mono-hydrogenated edge (H-edge) remain unaffected. Thus, the system develops a spin moment mainly localized at the H-edge. This property is not modified when the partially thiolated ribbon is attached to the gold substrate, and is quite independent of the width of the ribbon. Therefore, the *upright* adsorption of partially thiolated ZGNRs can be an effective way to decouple the spin-polarized channel provided by the H-edge from an underlying metal substrate [1]. These observations might open a novel route to build spin-filter devices using ZNGRs on gold substrates.

References

[1] Pepa Cabrera-Sanfelix, Andrés Arnau, Daniel Sánchez-Portal, Phys. Chem. Chem. Phys. 15 (2013) 3233-324

Figures



Magnetization density of a SAM-like arrangement of asymmetrically-thiolated ultrathin ZGNRs on Au(111) and the corresponding band structure, where the polarized edge-state has been highlighted.