Graphene-multiferroic heterostructures: electronic and magnetic properties by design

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Abstract

Spintronics is the new paradigm of information technology. The operating principle of the spin transistor [1] relies on the modulation of the current thanks to the Spin-Orbit (SO) Coupling in semiconducting materials and on spin injection *via* magnetized contacts. However the devices fabricated with conventional semiconductors suffer from short spin diffusion lengths and result in weak spin signals. C-based nanomaterials, instead, are considered highly promising for spintronic applications since can present spin diffusion lengths up to the 100 μm range and high electron velocity. However, a large spin diffusion length comes at the price of small SO coupling, which limits the possibility of manipulating electrons *via* an external applied field. In addition, to achieve graphene-based devices one also needs to open its vanishing electronic gap.

One way to open a band gap in graphene and preserve high carrier mobility is to put graphene on a suitable substrate. If, in addition, the substrate is insulating and magnetic, magnetism can be induced in the graphene sheet by proximity interaction [2, 3, 4]. Based on these considerations, we have investigated from first-principles an heterostructure consisting of the magnetoelectric (ferroelectric and magnetic) insulating $BaMnO_3$ [5] sandwiched between two graphene sheets [Fig. 1]. The ground state of $BaMnO_3$ is hexagonal and fits on the 4x4 graphene cell. The calculations have been performed using the SIESTA code in the local spin density (LDA) approximation, using a basis set and computational parameters optimized for the accurate modeling of ferroelectricity and magnetism in bulk $BaMnO_3$. In this framework we predict that the Mn atoms present an A-type antiferromagnetic order with spins antiparallel along the heterostructure direction and parallel in each layer. Magnetism is induced in the graphene sheets thanks to the high magnetic moment residing on the Mn atoms (~ 2.4 μ_B) and to the strong interaction between graphene and the Mn-terminated side of the slab. The spin density of the heterostructure, illustrated in Fig. 2, shows that the strongest magnetization is induced on the C atoms belonging to hexagons centered on the Mn atoms. Majority (black lines in Fig. 3) and minority (red lines in Fig. 3) carriers are characterized by quite different electronic properties: The band-gap for majority and minority carriers occurs, respectively, on the M-Γ line and at the K point, predicting an anisotropy between the two types of carrier. The electronic gap is inherited from the $BaMnO_3$. The graphene Dirac cones are into the valence band with a slope dependent on the spin type, hence producing a spin-depended carrier mobility in the whole heterostructure.

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References

[1] S. Datta and B. Das, Appl. Phys. Lett. **56** (1990) 665.
[2] M. Weser *et al*., Appl. Phys. Lett. **96** (2010) 012504
[3] H. Haugen, D. Huertas-Hernando, A. Brataas, Phys. Rev. B, **77**, 115406 (2008)
[4] H. X. Yang A. Hallal, D. Terrade, X. Waintal, S. Roche, and M. Chshiev Phys. Rev. Lett. **110** (2013) 046603.
[5] J. Varignon and Ph. Ghosez, Phys. Rev. B **87**, (2013) 140403(R)
[6] J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejon and D. Sanchez-Portal, J. Phys. Condens. Matter **14**, 2745 (2002)

Figures

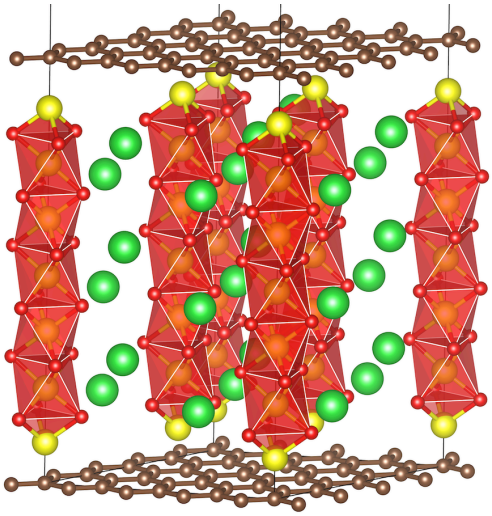

Figure 1. Ball-and-stick model of the heterostructure consisting of 13 monolayers of $BaMnO_3$ sandwiched between two graphene sheets. The color code is: Ba = green, Mn = yellow, O = red, C = gold.

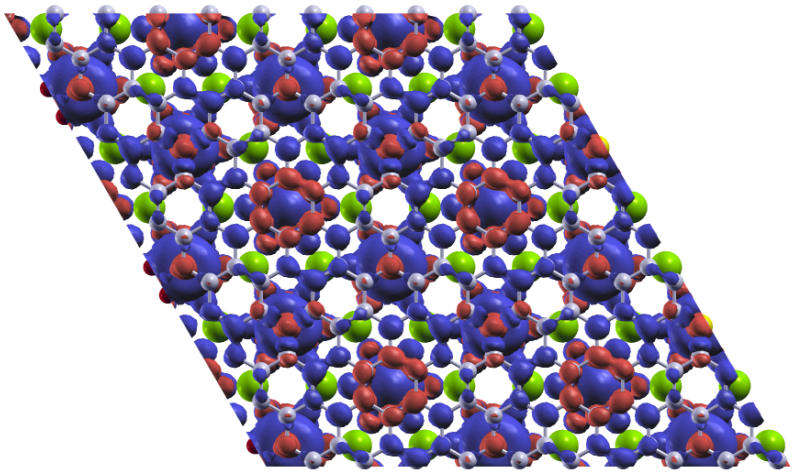

Figure 2. Spin density ($\rho\uparrow - \rho\downarrow$) of the hybrid graphene-$BaMnO_3$ system. Red and blue isosurfaces indicate majority and minority spin densities. The greatest spin polarization is induced on the C atoms belonging to the hexagons centered on Mn atoms.

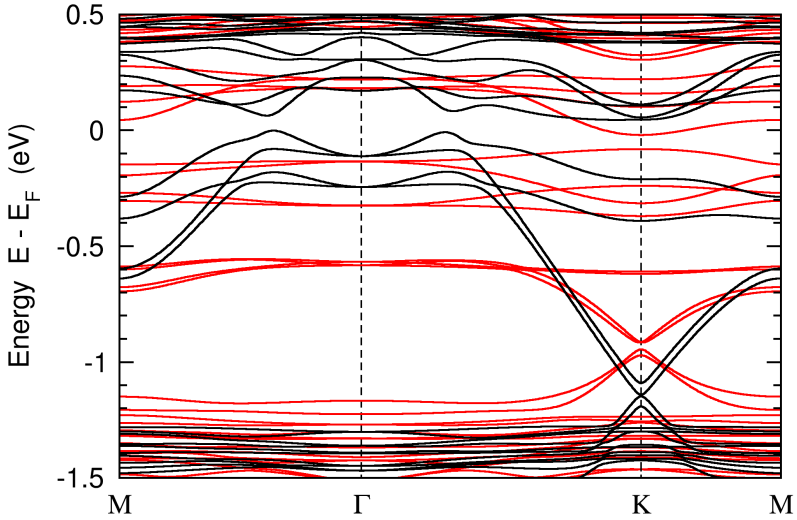

Figure 3 Spin-polarized electronic band structure of the graphene-BaMnO3 sandwich structure. Majority and minority spin channels are indicated with black and red lines. The graphene bands are duplicated due to the presence of two graphene sheets in the heterostructure. The Fermi level is used as a reference for the energy.