First-Principles Design of Novel Materials for Spintronics Applications

Motivation

Spintronics, or spin transport electronics, is a field of technology that exploits the electron spin, possibly in addition to the electron charge, to achieve the next generation of electronic devices. As magnetic effects occur at smaller energy scales than the electronic ones, spintronic devices promise low-power dissipation devices. Furthermore, as magnetic interactions are enhanced at the nanoscale, spin-based devices can also allow one to achieve device miniaturization.

Despite many active and passive spin-devices have been achieved, the quest for optimal materials for spintronics applications is still open. For instance, the Datta spin transistor [1] is based on the concept that it is possible to manipulate the spin of the electrons in the channel material via an external electric field, the ability to act on the spin being proportional to the Spin Orbit Coupling (SOC) of the material. For this, materials with simultaneously high SOC and long spin coherence length are sought for. However, these requirements are often in conflict: typical semiconductors present high SOC but short spin coherence length.

On the contrary, carbon nanomaterials have a remarkably long spin diffusion length (two order of magnitudes larger than in inorganic semiconductors) but extremely small SOC. Graphene presents an additional difficulty: it has a vanishing electronic band gap, which makes impossible to switch off a graphene-based transistor.

Computations

We propose to overcome both difficulties, weakness of the SO interaction and lack of a band-gap, by placing graphene on a magnetic semiconducting substrate. As representative of this family, we choose a hexagonal Mn-based magnetoelectic: BaMnO3. We have used first-principles techniques as implemented in the SIESTA code, to compute the structural, electronic and magnetic properties of the graphene/BaMnO3 interface [2]. The use of high-performance machines has been critical to address this material system, due to the large size (large number of atoms) needed to model various graphene/BaMnO3 slabs. Calculations have been performed on several machines: JUROPA/JURECA at FZJuelich (Germany) and LINDGREN at KTH (Sweden), as the work lasted three years.

Results

Using this approach, we have shown that the spin polarization is induced in the pristine carbon network [Fig. 1], exclusively due to the strong interaction between the Carbon π and the Mn d states (proximity interaction). Analysis of the electronic band structure shows that the effect is general and valid for any RMnO3 (with R a rare-earth material) compound. The resulting hybrid system is half-metallic: majority carriers present an electronic band gap, while minority carriers have no gap. Hence, the graphene-BaMnO3 can act as an injector of 100% spin polarized carriers. Since BaMnO3 is not only magnetic but also insulating, we suggest using a thin layer of such a material to simultaneously achieve spin injection and high resistance

contacts. This approach has the advantage of combining in one material – the magnetic insulator – the two main features of the most efficient injection scheme known to date: ferromagnetic contacts followed by a tunnel barrier of insulating material deposited on graphene [Han2014]. A possible device exploiting these results is a spin–FET in which spin injection is obtained by graphene-BaMnO3 in its ground state. Then, the FET channel can be made by graphene on an insulating material, such as hexagonal Boron Nitride (hBN), which preserves the long intrinsic spin coherence length of carbon. A high SOC substrate would enable control of the spin in the channel. The continuous graphene with a modulated substrate minimizes problems with contact resistances and interface mismatch in the transport direction.

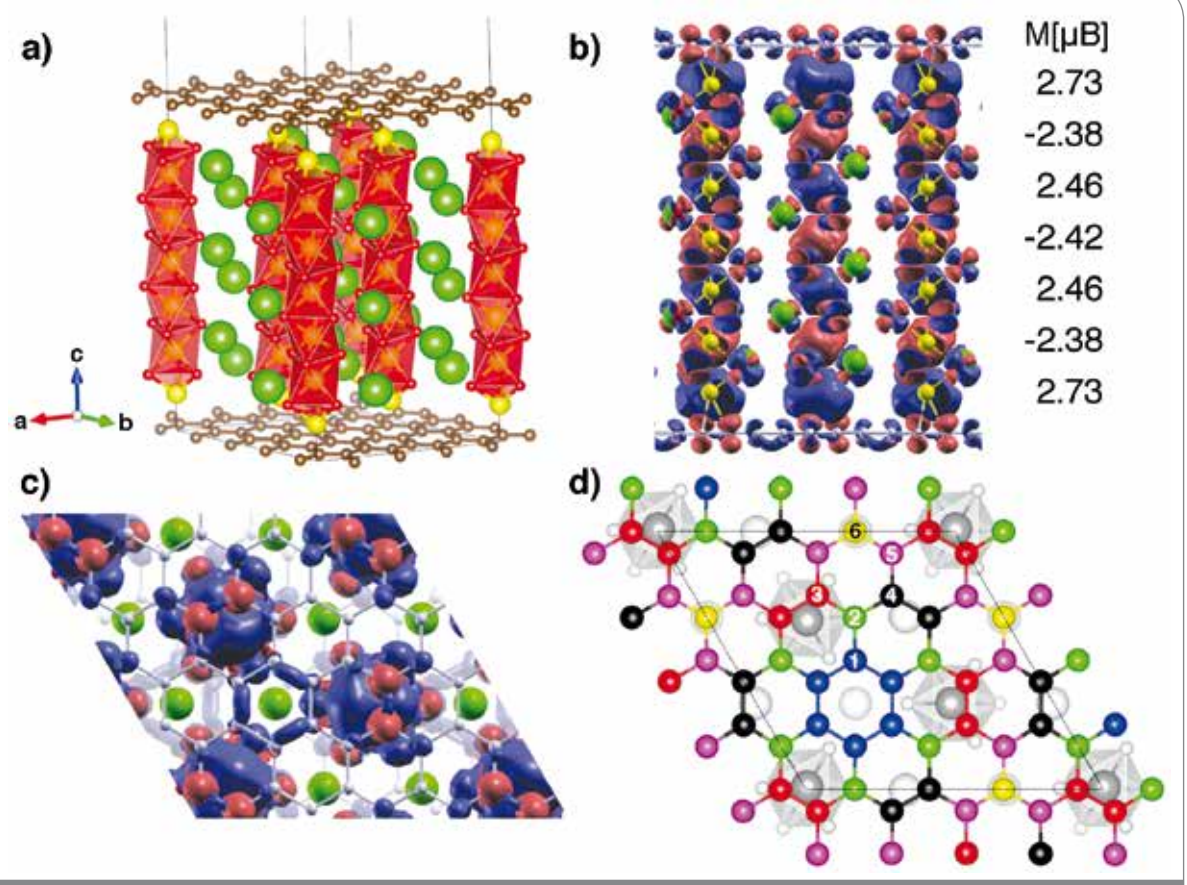

Fig. 1. Ab initio relaxed graphene–BaMnO3 structure (a) and the corresponding side (b) and top (c) view of the computed spin density (ρ↑ – ρ↓). Blue and red correspond to positive and negative isodensities, respectively. The magnetic moment on the Mn atoms are indicated in panel (b). The spin polarization induced on graphene is apparent in panel (c) The resulting six graphene sublattices are numbered and indicated with different colors in panel (d) [From Ref. 2]

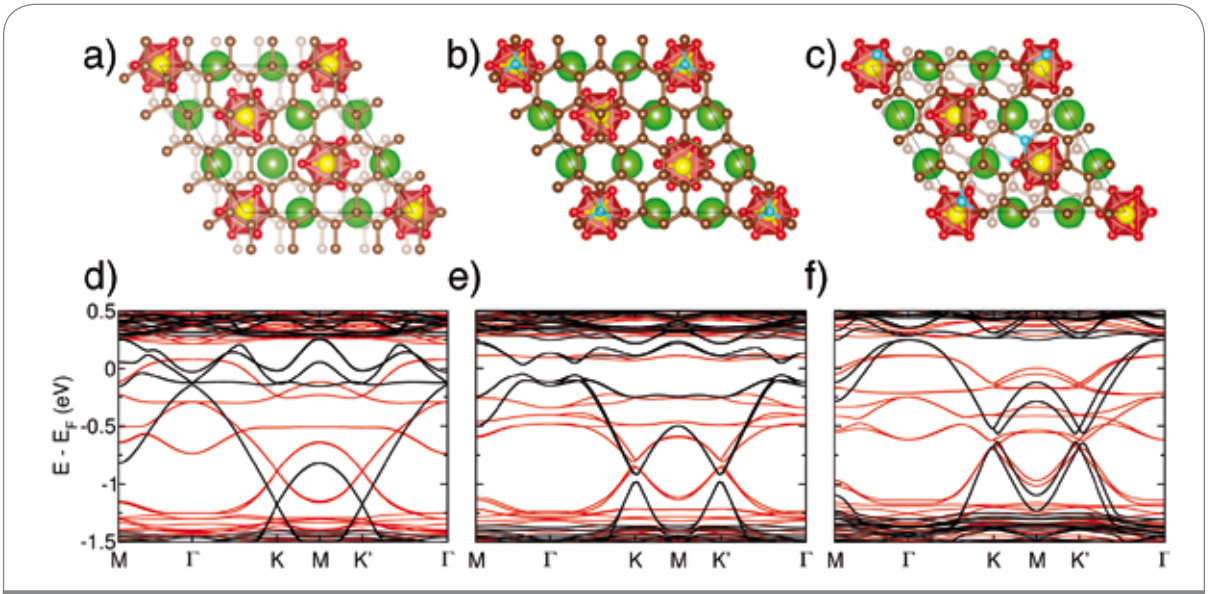

Fig. 2: Structural and electronic properties of the graphene–BaMnO3 slab. Ball-and-stick model (top) and electronic band structure (bottom) of graphene–BaMnO3 in its ground state (left), and of the relaxed structure with one (middle) and two (right) substitutional Boron atoms. The position of the Dirac cones is shifted towards the Fermi energy (EF) with increasing doping. Red and black solid lines indicate, respectively, majority and minority spin channels. The Fermi energy of the hybrid system is taken as a reference. Atom colors: Mn yellow, Ba green, O red, C gold, B light blue. [From Ref. 2]

Going further, our simulations show that the high-mobility region, characteristic of graphene electronic band structure, are preserved in the hybrid system. High-mobility is achieved when the energy has a linear dependence on the momentum, resulting in the so-called Dirac cones. The latter are found in the band structure and the splitting between majority and minority cones is quite large (~300 meV), but they occur at quite low energy. We address this issue by showing that doping of graphene with acceptors can be used to tune the Dirac cones, moving them into the experimentally accessible energy range [Fig. 2]. The velocity of the two types of carriers is quite different, so spin dependent transport is expected in this hybrid material.

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