Electronic and magnetic properties of graphene nanoribbons deposited on the topological insulator Sb_2Te_3

Wei Zhang[1,2], Farideh Hajiheidari[1], Yan Li[1,3], Manuel Schmidt[1], and Riccardo Mazzarello[1,4]*

[1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52074 Aachen, Germany
[2]Center for Advancing Materials Performance from the Nanoscale, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, PR China
[3] Institute IEK-6, Forschungszentrum Jülich, D-52425 Jülich, Germany
[4] JARA-FIT and JARA-HPC, RWTH Aachen University, D-52074 Aachen, Germany,
*mazzarello@physik.rwth-aachen.de

Three-dimensional Topological insulators (TIs) are a recently discovered class of band insulators having conducting surface states in the bulk band gap[1,2,3]. The surface states are topologically protected against non-magnetic disorder but magnetic perturbations have a profound impact on their properties. In this work we present a first-principles investigation of zigzag graphene nanoribbons (GNRs), which possess magnetic edge states in a free-standing configuration, on the (111) surface of the topological insulator Sb_2Te_3. We consider both unpassivated and H-passivated nanoribbons. We believe this system is an interesting candidate for an experimental investigation of proximity effects between a magnetic system and a TI. In principle, these effects could be exploited in spintronics devices integrating Tis with magnetic materials.

As a preliminary simulation, we study the structural and electronic properties of monolayer graphene on Sb_2Te_3 (111). We consider several configurations with different adsorption sites for C atoms and optimize their geometry. The most stable configuration turns out to be the hollow configuration. The presence of the TI induces a gap of about 20 meV at the graphene Dirac point and slight p-doping of graphene.

In the H-free case, the chemical interaction between the surface and the edges of the GNRs is very significant and the GNR is strongly bent, as shown in Fig. 1(a). The distance between edge C atom and the Sb_2Te_3 surface is 1.95 Å, while the distance at the center of the GNR and the Sb_2Te_3 surface is 4.72 Å. In spite of the pronounced interaction, edge magnetism is preserved. The effect of this relatively strong one-dimensional perturbation on the properties of the surface states is currently under investigation. We are also computing magnetic anisotropy energies.

Next, we consider H-terminated GNRs on Sb_2Te_3 (111). The equilibrium distance between the nanoribbon and the surface is larger, about 3.4 Å (see Fig. 1(b)). As a result, the electronic properties of the GNR are barely affected by the presence of the surface: the GNR exhibits edge magnetism with antiferromagnetic coupling between the two edges. Furthermore, the exchange interaction between the edge-state spins and the surface-state spins is very weak and the surface states do not display any energy gap but only a small shift of their Dirac point to lower energies.

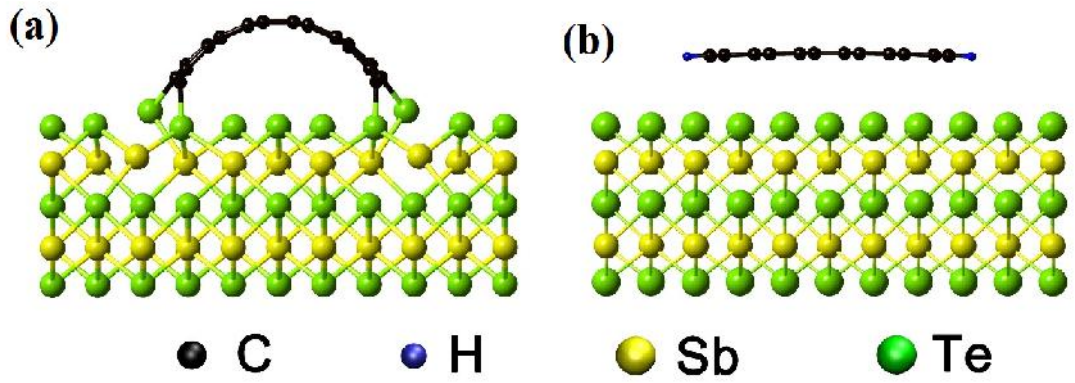

FIG. 1. (a)-(b) Side view of the relaxed models of H-free and H-terminated GNRs on Sb_2Te_3. Sb, Te, C, and H atoms are rendered with yellow, green, black and blue spheres.

The structural optimization and the calculation of the electronic properties were carried out using the plane-wave package Quantum-Espresso [4], a plane-wave package based on Density functional theory (DFT).

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