First-principles study of graphene nanoribbons deposited on the topological insulator Sb_2Te_3

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Three-dimensional topological insulators (TIs) are a recently discovered electronic phase of matter, which originates from strong spin-orbit interaction and time-reversal symmetry [1]. These materials possess conducting surface states in the bulk band gap. The surface states show remarkable properties, including spin-momentum locking and a linear energy-momentum dispersion, which can be described by an effective two-dimensional Dirac equation. Furthermore, these states are robust with respect to disorder, as long as it does not break time-reversal symmetry.
In this work, we explore the possibility of using zigzag graphene nanoribbons (GNRs), which possess spin-polarized edge states, to break this symmetry. We present a thorough study of the structural, electronic and magnetic properties of GNRs deposited on the (111) surface of the TI Sb_2Te_3 by first-principles methods based on Density Functional Theory. We employ gradient-corrected density functionals, in combination with semi-empirical van der Waals corrections. We consider unpassivated GNR edges, which bind strongly to the substrate. We show that the edge magnetism is preserved, in spite of the strong interaction between the edge carbon atoms and the TI surface. Furthermore, the coupling between the two edges is shown to be antiferromagnetic, as occurs for free-standing GNRs. Our results indicate that GNRs on Sb_2Te_3 are promising candidates for an experimental investigation of proximity effects between a magnetic system and a TI [2].

References

[1] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98** (2007) 106803.
[2] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82** (2009) 3045.

Figures

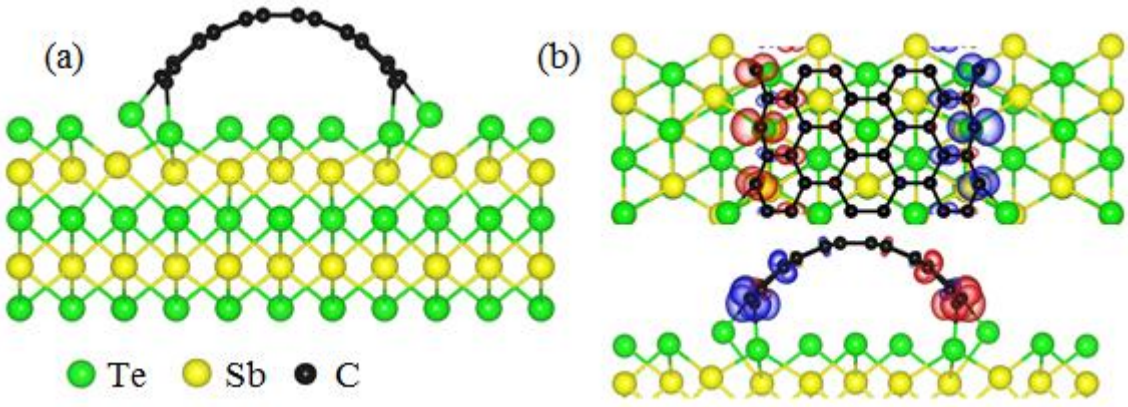

Figure 1: (a) Side view of the H-free GNR deposited on Sb_2Te_3 after relaxation. (b) Top and side view of an isovalue surface of the edge state spin density of the deposited GNR.