Ab-initio study of H-terminated and H-free zigzag graphene nanoribbons deposited on the surface of topological insulator Sb_2Te_3

Abstract:

Magnetism in zigzag graphene nanoribbons (GNRs) has received enormous attention recently, due to the one-dimensional nature of this phenomenon, as well as its potential applications in the field of spintronics. In this work, we present a density functional theory (DFT) investigation of zigzag graphene nanoribbons, 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. In the H-terminated case, the chemical interaction between the GNR and the substrate is weak. As a result, doping effects are almost negligible, and the mean-field magnetic properties of the GNR are preserved. In contrast to mono-hydrogenated GNRs, unpassivated edges bind strongly to the substrate. The interplay between strong spin-orbit coupling (SOC) and broken inversion symmetry lead to chiral configurations in low-dimensional magnetic systems deposited on heavy-element surfaces. This phenomenon is due to the Dzyaloshinskii-Moriya interaction (DMI), which favours non-collinear magnetic structures. In the H-free case, this interaction leads to a twisting of the two antiferromagnetically-coupled edge states of a zigzag graphene nanoribbon deposited on Sb_2Te_3. The resulting net magnetization shifts the Dirac point of the surface state of the TI and can even open a small gap depending on its direction. To our knowledge, this is the first report of a chiral magnetic structure formed by these one-dimensional states. The presence of a finite total magnetization could lead to applications of GNRs as spin filters in graphene-based spintronics devices.