Interfacing 2D materials with a ferrite: Gr/Fe_3O_4(111) and MoS_2/Fe_3O_4(111)

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Heterostructures consisting of half-metals, e.g. spinel metal oxides (MOs) and 2D materials (2DMs) are considered the future of spintronics, i.e. electronics in which the spin of an electron, and not only the charge, is utilized for information transfer and storage. They may also find application in valleytronics, which is electronics based on the local minima in electronic band structure. Among spinel MOs, Fe_3O_4 (magnetite) is known to exhibit high spin polarization at the Fermi level, making it a promising spin-filtering material (a material generating current of electrons with a certain spin). However, in a spintronic device, the generated spin-polarized current has to be transferred from one component to the other. With this respect, epitaxial graphene (Gr) – with its high spin diffusion length – is a perfect bonding element. When it comes to valleytronics, combing high spin polarization MOs with molybdenum disulfide (MoS_2) – a well-known valleytronic 2DM – should provide routes for valleys' polarization. Though, before these ambitious goals can be achieved, fundamental studies aimed at determining the structure and properties of various 2DM/MO systems have to be performed.

We have used spin-polarized DFT+U to study two 2DM/MO system: Gr/Fe_3O_4(111) and MoS_2/Fe_3O_4(111). In the calculations, the most common surface termination of Fe_3O_4(111), the Fe_{tet1}, was applied. Gr was place on Fe_3O_4(111) in a (√3×√3)R30° supercell, with Gr layer stretched by about 5.2%. Even though two possible layer's positions are characterized by the same adhesion energy, equal to –0.46 eV/Å, they differ in electronic structure. When one of the carbon atoms is placed just over the topmost iron atom (Fig. 1b), there is no band gap at the Fermi level. On the other hand, when there is no direct C-Fe interaction, a band gap for spin-up electrons appears. The graphene is *n*-doped through charge transfer from iron, thus, the Dirac cones are moved below the Fermi level by about 0.47/0.37 eV. Surprisingly, these cones are spin-split by about 0.13 eV. In separate calculations, the T2 phase of MoS_2 was adsorbed on Fe_3O_4(111) in a (1×1) cell (without any rotation). Sulphide's distance to the substrate was found to be relatively big (2.183 Å), with the layer remaining flat. This indicates weak interaction with the oxide. Interestingly, magnetic moments on topmost tetrahedral Fe atoms change their sign and value from -3.998 to +3.847 μ_B.

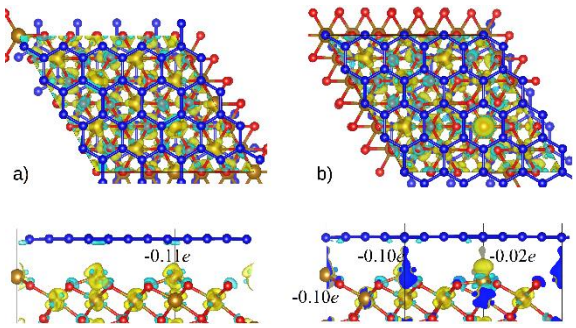

Fig. 1. Charge density difference for two different (√3×√3)R30° adsorption geometries (shown in *a* and *b*) of Gr on Fe_3O_4(111) (top and side views). The numbers indicate Bader charges on Fe topmost atoms. The isosurfaces show charge density changes. Golden, red and blue balls represent Fe, O and C atoms, respectively.

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