ELECTRONIC AND MAGNETIC PROPERTIES OF THE GRAPHENE-FERROMAGNET INTERFACES: *AB INITIO* SIMULATION

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Graphene is a two-dimensional sheet of carbon atoms arranged in a honeycomb lattice with two crystallographically equivalent atoms (C1 and C2) in the unit cell [1, 2]. The sp^2 hybridization between one *2s* orbital and two *2p* orbitals leads to a trigonal planar structure with a formation of a σ bonds between carbon atoms that are separated by 1.42 Å. These corresponding σ bands have a filled shell and, hence, form a deep valence band. The half-filled $2p_z$ orbitals, which are perpendicular to the planar structure, form the bonding (π) and antibonding (π^*) bands in the electronic structure of graphene. The π and π^* bands touch in a single point exactly at the Fermi energy (E_F) at the corner of the hexagonal graphene's Brillouin zone (K-points). Close to this so-called Dirac point (E_D) the bands display a linear dispersion and form perfect Dirac cones [3]. Thus, undoped graphene is a semimetal ("zero-gap semiconductor"). The linear dispersion of the bands mimics the physics of quasiparticles with zero mass, so-called Dirac fermions [1 - 3].

The exceptional transport properties of graphene make it a promising material for application in microelectronics [4]. This has recently led to a revival of interest in graphene on transition metal surfaces [5, 6], as large area epitaxial graphene layers of exceptional quality can be grown, which might be an alternative to micromechanical cleavage for producing macroscopic graphene films.

The electronic interaction of graphene with a metal is both of fundamental and technologicalinterest in view of possible device applications. Graphene might be the best material for the realization of spintronic devices. Such systems usually require the effective injection of the spin-polarized electrons in the conductive channel which can be made from graphene [7]. However, prior to being able to implement graphene/ferromagnet systems in any kind of spintronic unit, a study of their electronic, magnetic, and interfacial properties has to be performed. Binding between graphene and metallic surface can be either chemical or physical in nature.

Chemical binding typically implies a strong interaction through a charge sharing between the substrate and the adsorbate, yielding modification of their electronic structures. Physisorption, on the other hand, arises due to classical electrostatic or dispersion (van der Waals) interactions.

The electronic and structural properties of the graphene-substrate system are obtained using the Perdew-Burke-Ernzerhof (PBE) functional [8]. For solving the resulting Kohn-Sham equation we have used the Vienna Ab Initio Simulation Package (VASP) [9, 10]. The plane-wave kinetic energy cutoff is set to 520 eV. The supercell used to model the graphene-metal interface is constructed from a slab of 7 layers of metal atoms with a graphene sheet adsorbed at both sides and a vacuum region of approximately 15 Å. When optimizing the geometry, the positions (z-coordinates) of the carbon atoms as well as those of the top two layers of metal atoms are allowed to relax. In the total energy calculations and during the structural relaxations the k-meshes for sampling the supercell Brillouin zone are chosen to be as dense as 21 × 21 and 11 × 11, respectively.

The electronic structure and magnetic properties of the graphene/ferromagnet interface were investigated via theoretical methods (DFT functional). The different interfaces were analyzed: graphene/Ni(111), graphene/Co(0001) . Here the electronic structure of the interface as well as the effect of induced magnetism in graphene layer were discussed. In all cases a strong modification of the electronic structure of the graphene layer and FM substrate upon graphene adsorption were detected in theoretical calculations. This modification is due to the considerable hybridization of the graphene π and FM *3d* valence band states accompanied by the partial charge transfer of spin-polarized electrons from FM onto C atoms leading to the appearance of the effective magnetic moment in the graphene layer.

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