Substrate-induced magnetism in epitaxial single layer graphene

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Of particular intereSt is the magnetism of the single layer graphene (SLG). As we know published experimental data on a ferromagnetism of materials based on graphene in the paper [1] only are presented. The authors [1] suppose that the ferromagnetism at the room temperature is caused by defects of graphene. We have studied the band structure as well as magnetic properties in the ferromagnetic heterointerface SLG/MnO(001) using *ab initio* calculations.

We have modeled the SLG/MnO(001) ultra-thin film by a slab using a supercell approach with periodic boundary conditions. The slab included four-six layers containing 33 - 153 atoms in the supercell and each slab was separated from the other by a vacuum region. The band structure calculations were performed using the self-consistent plane-wave pseudopotential method within the framework of DFT. On the basis of the atomic effective charge concept estimations of the value Q_{eff} have been performed. The estimations analysis permits to calculate a charge transfer to the bond Mn – O that amounts ~ 0.50*e*. It is possible to suppose that an additional charge transfer from the manganese atoms to the carbon atom exists and amounts ~ 0.04 e.

Our estimations of the magnetic moment value at carbon atoms have shown that the total magnetic moment of the graphene islet formed by 28 atoms amounts $0.28\mu_B$. The analysis shows that the little magnetic moment at carbon atom amounts: ~ 0 μ_B (14%); 0,01 μ_B (58%); 0,02 μ_B (21%) and 0,03 μ_B (7%). Due to the band structure analysis of the system SLG/MnO(001) above we have drawn a conclusion of the C*2p*-Mn*3d*-hybridization formation of free and filled states. As a result of the *pd*-hybridization an orbital energy of free electron *2p*-states of carbon in graphene lowers that reduces to these states admixture to valent *3d*-states of manganese in the ultrathin layer MnO(001) and to Fermi surface topology change. This circumstance may be responsible for the "flickering" magnetism formation in graphene of the system SLG/MnO(001). Noteworthy that in graphene the magnetism revealed in the present paper is induced by the substrate MnO(001) as the *pd*-hybridization result.

Several laSt carbon atoms ("zigzag" type) of the graphene islet turn out to be nonmagnetic and within the bounds of the authors' concept [2] one can suppose that these atoms have a sp^3-configuration as well as take part in a bond formation with the substrate.

Therefore the obtained data on the magnetism nature in the ferromagnetic heterointerface SLG/MnO(001) can be considered as the possible base for implementations in spintronics devices.

[1] Y. Wang, Yu. Huang, Y. Song. *Nano Lett.* **9**, 220 (2009).
[2] A. Ramasubramaniam, N.V. Medhekar, V.B. Shenov. *Nanotechnology* **20**, 275705 (2009).