First-principle study of functionalized graphene.

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Abstract

Surface electron structure is insufficiently studied phenomenon. In this respect, graphene is an ideal object not only due to the expectations of breakthroughs in microelectronics and materialogy based on carbon materials, but also because graphene is suitable object for the surface phenomena study. Recent studies have shown that the greatest practical interest is not "ideal" structure of graphene, but rather its defects. Numerous studies have shown high sensitivity of graphene electron and its energy structure to defects of various kinds [1], including the atoms adsorbed on its surface, thus confirming that the chemical modification of graphene is a promising direction of the management of its electronic structure. Due to the fact that a significant portion of the above studies made on the basis of the pseudopotential method, it is of interest to study the changes in the electronic structure of graphene with the density functional theory (DFT) on the basis of the full-potential wave function using linearized augmented plane wave method (FP-LAPW). Research was conducted with Elk Code package, exchange and correlation energies were evaluated with the local density approximation (LDA). For integration procedure in reciprocal space k-point mesh with different dimensions depending on the desired accuracy and acceptable calculation duration was used. Iteration process continues as long as the difference between the values of the total energy of the cell does not exceed 2 * 10-5 Ry. To calculate the integral spin magnetic moments of each atom, integration of the electron density for the two spin projections was held separately.

The results of changes in the electronic structure and magnetic properties of graphene at various number of adsorbed atoms of hydrogen and fluorine were presented. It was confirmed that the adsorption of atoms leads to a substantial change in the electronic structure of graphene and the appearance of the band gap in it, whose value depends on the impurity concentration. It is found that the magnetic properties of graphane and fluorographene depend on the distance between adjacent atoms adsorbed, and the distance between the fluorine atom and its associated carbon atom in the lattice of graphene. The features of the band structure and the electron density as a function of fluorine concentration and the degree of deformation of the graphene planes during the adsorption of fluorine were studied. The effect of the concentration of adsorbed fluorine as a factor of mutual influence of interaction between neighboring fluorine atoms on the electron graphene structure (C2F, C4F and C18F) was shown. Despite the similarity of DOS diagrams of C18F, C4F and C2F, following differences in C18F fluorographene were discovered:

- a significant reduction in the band gap size;
- the appearance of two peaks in the structure of the DOS near the Fermi level and the almost complete absence of dispersion of the line at 23 eV;
- emergence of many bands in the valence area of the band structure.

This is confirmed by similar changes in the structures in cases of spin polarization: a decrease in the concentration of fluorine reduces the size of the gap in the spectrum of electron structure and electron density in the diagram. Accordingly, the magnetic moment of C4F is reduced compared to C2F.

Research of influence of bond deformation conducted on C18F and C2F by changing the distance between the atoms C and F. Adsorption of fluoride on graphene leads to deformation of bond between neighboring carbon atoms due to the elevation of one atom above the flat graphene lattice. The easiest way to study changes in the electronic structure at various bond energies of C-F is by altering the distance between the atoms of fluorine and its associated carbon atom.

It is shown that the magnetic properties of graphane and fluorographene depend on the distance between adjacent atoms adsorbed, and the distance between the fluorine atom and its associated carbon atom in the graphene lattice.

References.

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