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Electronic and Magnetic Properties of the 8-ZGNR/h-BN(0001) Interface

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The results of a density functional theory investigations of structural and electronic properties of zigzag graphene nanoribbons 8-ZGNR/ h-BN(0001) are presented. The peculiarities of the spin state at the Fermi level and the role of the edge effect and the effect of substrate in formation of the band gap (380 meV) in 8-ZGNR/h-BN(0001) system were determined. The contributions of nanoribbon edges and the substrate in formation of the gap have been differentiated. The estimations of local magnetic moments on carbon atoms of the 8-ZGNR nanoribbon are made.

Keywords: Band structure, Hexagonal boron nitride, Graphene nanoribbons, Magnetic moments, Electronic properties.

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1. INTRODUCTIONS

Since its discovery in 2004, graphene attracts focused attention of researchers due to its unique properties [1]. High carrier mobility in graphene at room temperature opens a wide range of its practical applications for production of spintronics components and devices. However, there is a problem: zero energy gap in the band spectrum of graphene. The fact prevents graphene from being used in semiconductor devices. Known solutions to the problem employ graphene nanoribbons [2].

This paper studies the roles of the edge and substrate effects of zigzag graphene nanoribbons on electronic structure of the 8-ZGNR / h-BN(0001) interface as a component of spintronics devieces using ab initio the density functional theory (DFT).

2. MODEL AND METHOD

2.1 The Interface Model

The 8-ZGNR / h-BN(0001) interface model is based on three-dimensional periodic plate scheme. To simulate a system consisting of substrate and 8-ZGNR, we used a supercell containing unit cells of (4 × 4) h-BN and (4 × 4) graphene arranged within a plane (0001). The supercell parameter was selected to be divisible by the equilibrium value of the graphene unit cell parameter. Graphene cells were used to build a zigzag graphene nanoribbon (8-ZGNR). Fig. 1 demonstrates a fragment of the 8-ZGNR / h-BN(0001) plate. The surface and the 8-ZGNR / h-BN boundary was simulated as a plate consisting of three atomic layers of hexagonal boron nitride and a monolayer of zigzag graphene nanoribbon positioned at the distance of the d_0 bond. The basic supercell consisted of 90 atoms, each plate was isolated from others by 15 Å vacuum space.

2.2 Method

Band structure calculations were performed using the Quantum Espresso [3] software suite based on the density functional theory [4]. Plane waves and pseudopotentials were used as the fundamental calculation basis. Crystal periodic structure is accounted for using the unit cell boundary conditions. Nonlocal exchange correlation functionality was used in Perdew-Burke-Ernzerhof (PBE, PBEsol) parametrization. The plane waves cutoff energy for self-consistent field (SCF) calculation was 410 eV. Accomplished total cell energy convergence was at least 10^{-4} Ry/cell. To integrate linear Brillouin zone (BZ), 18 points in reciprocal space were used. Electron density calculations were made in spin-polarized variation for 8-ZGNR with ferro- and antiferromagnetic ordering.

3. RESULTS AND DISCUSSION

3.1 Atomic Structure

To study the atomic structure of the 8-ZGNR / h-BN(0001) interface, relaxation of graphene nanoribbon and one upper boron nitride atomic plane of the plate was performed. Two lower layers of the h-BN (0001) substrate were "frozen". Relaxation was carried out until the sum total of all forces in the system was reduced below 0,001 eV/Å. We established equilibrium parameter values for the lattices, atomic positions of the nanoribbon and the upper layer of boron nitride, and the length of the d_1 bond between the nanoribbon and substrate atomic layers. Results of DFT calculations for the 8-ZGNR / h-BN (0001) equilibrium system are summarized in Fig. 1b. Equilibrium bond length for 8-ZGNR and h-BN (0001) substrate was $d_1 = 0.339$ nm. Table 1 contains comparison of the parameters calculated for the 8-ZGNR / h-BN(0001) system with known data. In the examined configuration, the $d_{C\text{-}C}$ bond length between the carbon atoms in graphene nanoribbon amounted to 1,42 Å.

3.2 Band Structure

The band structure of the 8-ZGNR / h-BN(0001) interface with antiferromagnetic ordering is shown in Fig. 2. For this magnetic ordering patterns the role of

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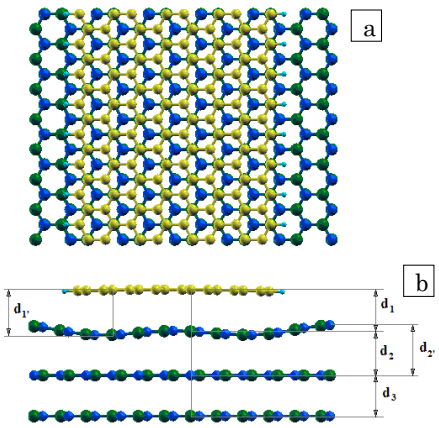

Fig. 1 – Atomic structure of 8-ZGNR / h-BN(0001): a – top view, b – front view

spin polarization becomes evident and demonstrated by greater opening of the energy gap for the spin down electron subsystem. As Fig. 2 demonstrates, energy gap Eg > 380 meV is typical of antiferromagnetic ordering in nanoribbons with zigzag edges using the 8-ZGNR / h-BN(0001) interface. Analysis of the data allows to differentiate to a certain extent the contributions of the nanoribbon edge and the substrate in the opening of the energy gap in the 8-ZGNR / h-BN(0001) system (with antiferromagnetic ordering).

Layout of the zones corresponding to 8-ZGNR to a large extent remains unchanged in the 8-ZGNR-AF / h-BN(0001) system, in particular, location and the shape of σ-bands and π-bands responsible for conductivity. However, some changes in 8-ZGNR states under the substrate influence are observed in the immediate vicinity of the Fermi level.

3.3 Magnetic Properties

The estimations of local magnetic moments on carbon atoms of the 8-ZGNR nanoribbon are made. It is to be noted that in nanoribbons 8-ZGNRs the edge oxygen atoms possess maximal local magnetic moments (0.27 μ_B) relative to central carbon atoms (0.02 μ_B). The edge carbon atoms in nanoribbon 8-ZGNR with antiferromagnetic ordering have opposite directions of magnetic moments. The nature of distribution of local magnetic moments on carbon atoms in zigzag graphene nanoribbons is in qualitative agreement with known data.

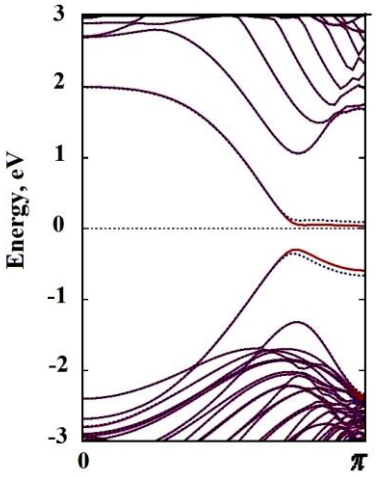

Fig. 2 – DFT band structure of 8-ZGNR / h-BN(0001) with antiferromagnetic ordering for both spins: red-spin up and blue-spin down. Fermi energy is assumed to be zero-point energy

4. CONCLUSIONS

Analysis of the dispersion characteristic of the 8-ZGNR-AF / h-BN(0001) interface in the vicinity of the Fermi level has demonstrated that within the PBEsol approximation appearance of an energy gap between the binding and antibinding π-regions of graphene nanoribbon is induced. Dispersion in the proximity of the Fermi level, just like the energy gap width, depended largely on the nanoribbon edge effect and varied from linear to parabolic. Appearance of an energy gap of about 380 meV in the 8-ZGNR-AF / h-BN(0001) interface with antiferromagnetic ordering opens certain opportunities for its use in components of graphene field-effect transistors and spintronics devices.

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