AB-INITIO SIMULATION OF HYDROGENATED GRAPHENE PROPERTIES

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I. INTRODUCTION

Graphene has been the subject of many recent investigations due to its peculiar transport properties [1]. But investigations are shown the problem connected with the lack of a graphene bandgap, which prevents its use in digital electronics. Chemical modification of graphene named as graphane has recently entered for investigation as possible candidate to solve this problem [2-3]. Graphane is the compound, which consist from two-dimensional graphene covalently bonded by some atoms of the hydrogen. Graphane is a semiconductor, which have of novel structure and low dimensionality. It provides a fertile playground for fundamental science and technological applications. To this purpose, in this work, main task is to investigate parameters and characteristics of the hydrogenated graphene by the ab-initio method.

II. METHOD AND PECULIARITIES OF SIMULATION OF HYDROGENATED GRAPHENE PROPERTIES

Ab-initio calculations have been performed by means of the Quantum Espresso [4] code, using the Perdew-Burke-Ernzerhof (PBE) parametrization of the generalized gradient approximation (GGA). A 40 Ry wave function cutoff and 240 Ry charge density cutoff have been considered, while the Brillouin zone has been sampled using a 24 x 24 x 1 Monkhorst–Pack grid. A 20 bohr layer of vacuum is considered to separate the sheet from its periodical images. We have extracted the effective mass and other parameters from results of the density functional theory DFT-GGA simulations.

III. RESULTS OF MODELING OF PARAMETERS AND CHARACTERISTICS OF THE HYDROGENATED GRAPHENE BY THE AB-INITIO METHOD

Relaxed structures for 100% and 50% hydrogenated and fluorinated graphene (from here on H100%, H50%, F100%, and F50%, respectively) are in agreement with results already shown in the literature [2-3]. We show some results for the considered H50% and H100% structures in Figures 1 and 2. Figure 1, a shows the peculiarities of the arrangement of carbon (C) and hydrogen (H) atoms and figure 1, b - the zone diagram in the structure of 50% hydrogenated graphene (or graphane of C2H1 type).

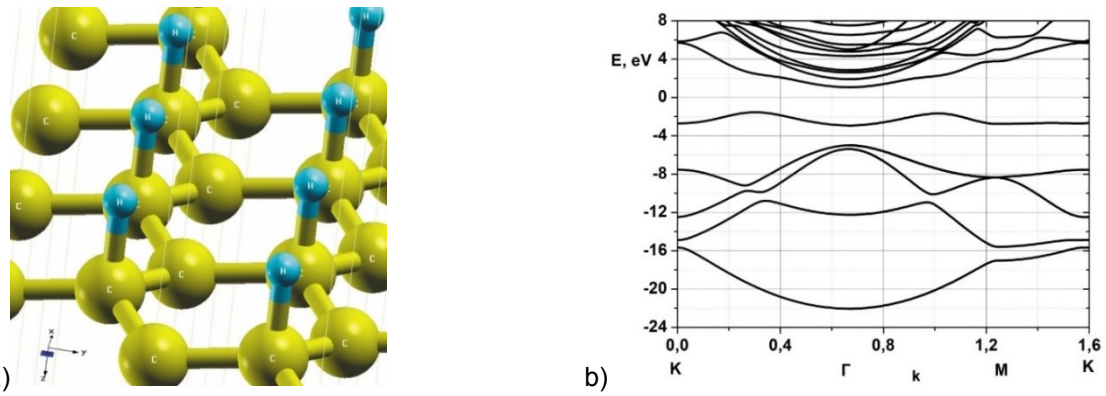

Figure 1. a) Features of arrangement of carbon (C) and hydrogen (H) atoms and b) zone diagram in the structure of 50% hydrogenated graphene (graphane of C2H1 type)

Figure 2, a shows the peculiarities of the arrangement of carbon (C) and hydrogen (H) atoms and figure 2, b - the zone diagram in the structure of 100% hydrogenated graphene (or graphane of C2H2 type). From the

analysis of this figures, which shows the dependences of the energy values E (eV) on the normalized value of the wave vector k, it is clear that the hydrogenated graphene is characterized by a three-valley Γ-M-K band diagram. Valley Γ is characterized by the smallest energy gap between the conduction and valence bands. When modeling the electronic characteristics and parameters of hydrogenated graphene it is necessary to analyze the parameters of all three valleys K, M and Γ.

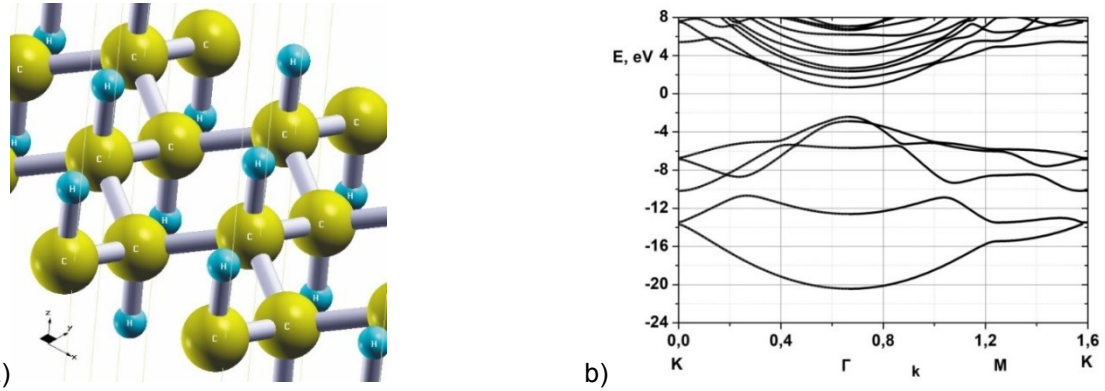

Figure 2. a) Features of arrangement of carbon (C) and hydrogen (H) atoms and b) zone diagram in the structure of 100% hydrogenated graphene (graphane of C2H2 type)

Effective electron masses for graphane of C2H1 and C2H2 have been calculated taking into account the value of the parameter E_g, which is the energy gap between the conduction and valence bands for the Γ-M-K valleys.

IV. CONCLUSIONS

Modeling of electron transfer processes in three-dimensional semiconductor structure containing graphane is carried out. We have extracted the effective mass and other parameters from results of the density functional theory DFT-GGA simulations. Due to the use of graphane with such characteristics of transfer of charge carriers it is possible to achieve a graphene transistor structure with open bandgap. The high mobility and high speed of charge carriers make graphene a promising material for creating new semiconductor devices with good output characteristics.

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