AB INITIO CALCULATION Al, Co, Sr DOPED GRAPHEME

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This paper introduces the results of first-principle calculations of the electronic and magnetic properties of graphene doped by Al, Co, Sr. In according to theoretical calculations by doping Co and Al graphene energy gap is opened. Furthermore, substitution of the Sr atom for a carbon atom in graphene increases magnetization. In addition, density of state was explored for Al, Co, Sr atoms doping of the graphene structure.

Keywords: first-principle calculations, DFT, ATK, graphene, Al, Co, Sr-doped, supercell, DOS, magnetic moment.
PACS: 31.10. +z, 31.15.E-, 75.50.Gg.

INTRODUCTION

Graphene is a zero band gap semiconductor or semimetal which consists of an sp^2 hybridized single atomic layer of carbon atoms organized in a hexagonal lattice. Each of tetravalent carbon atoms, connect to three neighboring atoms by covalent bonds, which left a free electron on each carbon atom. These free electrons lead to the high electron mobility and high conductivity of graphene. Graphene has also the advantage of being atomically thin conductive material [1-4].

Ferromagnetic properties for alkaline earth doped graphene such as Mg-graphene, Sr-graphene and Ba-graphene were predicted [5]. The calculations are devoted to the evaluation of electric properties of zigzag graphene nanoribbons influenced by the doping of Co [6,7] and Au [8]. Many studies about transition metal incorporated with armchair graphene nanoribbons have been conducted, such as Mn [9], Fe [10], and Ni [11]. In [6] reported an *ab initio* study of atomic and electronic structure of Co atoms incorporated in graphene nanoribbon with armchair-shaped edges.

In according to the electronic, optical, thermal, magnetic, mechanical and electrochemical properties of graphene become attractive for studying in various fields of research, such as electronics [12], optoelectronics [12,13], energy conversion and storage devices [14,15], sensors [16,17] and biomedicine [18,19]. In [20] have overviewed recent methods adopted to the electronic and magnetic properties of graphene and the possible practical applications of these methods in various areas of research. In addition, the challenges faced by individual methods are also included.

The energy gap (E_g) of Al doped graphene [21] is opened upon adsorption of (CO, CO_2, NH_3, NO, NO_2 and SO_2) in various way. The Al doped graphene with NO gas adsorption has the ability to donate electron; it needs to small energy to remove an electron to become a cation. To overcome the insensitivity of these molecules on pristine graphene, doped graphene will be appreciated because of the formation of a 3D structure. It is set that doping graphene with metals the higher sensitivity of graphene toward different molecules could be achieved [22–24]. Doping causes an improvement in the electronic behavior of the semiconductor materials. For instance, behind doping with B or N atoms, graphene expanded into p-type or n-type correspondingly [25]. Theoretical studies demonstrated that the doped atom on graphene could transform the band structure as well as the electron transfer so the applications of graphene could be mainly enhanced [26–28]. Among diverse metals, Al, Ag, Cu, Au, and Pt are the atoms which have been the most utilized for the doping of graphene [29]. By doping graphene with Al, the electron density around the doped atom reduces because of catching electron by surrounding C-atoms.

COMPUTATIONAL DETAILS

The electronic properties of vacancy in graphene was studied by the density functional theory (DFT) method within the Generalized Gradient Approximation (GGA). The band structure (BS) and density of states (DOS) have been calculated. DFT have been performed to explore the electronic and magnetic properties of graphene doped Al, Co, Sr. The magnetic moments calculation were down by Mulliken population analysis.

First-principles calculations based on the spin-polarized density functional theory, were performed using the periodic Atomistix Tool Kit (ATK). The generalized gradient approximation in the Perdew–Burke–Ernzerhof (PBE) parameterization was employed for the exchange–correlation functional. The kinetic cut-off energy was 150 Ry. The primitive cell of Graphene was relaxed and optimized with force and stress tolerances of 0.01eV/Å and 0.01eV/Å^3, respectively. A 4 x 4 x 1 k point was used for geometry optimization and total energy calculations. Our calculations were performed for a number of supercells with as many atoms as 18.

Al, Co, Sr-DOPED IN GRAPHENE

In result of our theoretical calculations we observed that energy gap opening of graphene by doping Co and Al. We calculated the energy gap for Co and Al is E_g=0.76eV, E_g=0.375eV respectively. Figure 1 displays the Projected Density of States

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(PDOS) which was constructed for s-, p- and d- electrons of Al atom in the 18-atom graphene supercell. The upper curve correspond to electrons with the direction of the spin up and the lower the direction of the spin down. Ab initio calculation PDOS for graphene showed that Fermi level for the p, s, d- electrons with spin-up and spin-down are almost similar [Fig. 1 b,c,d]. In figure 1-d is shown for the spin-down and spin up d- state below Fermi level.

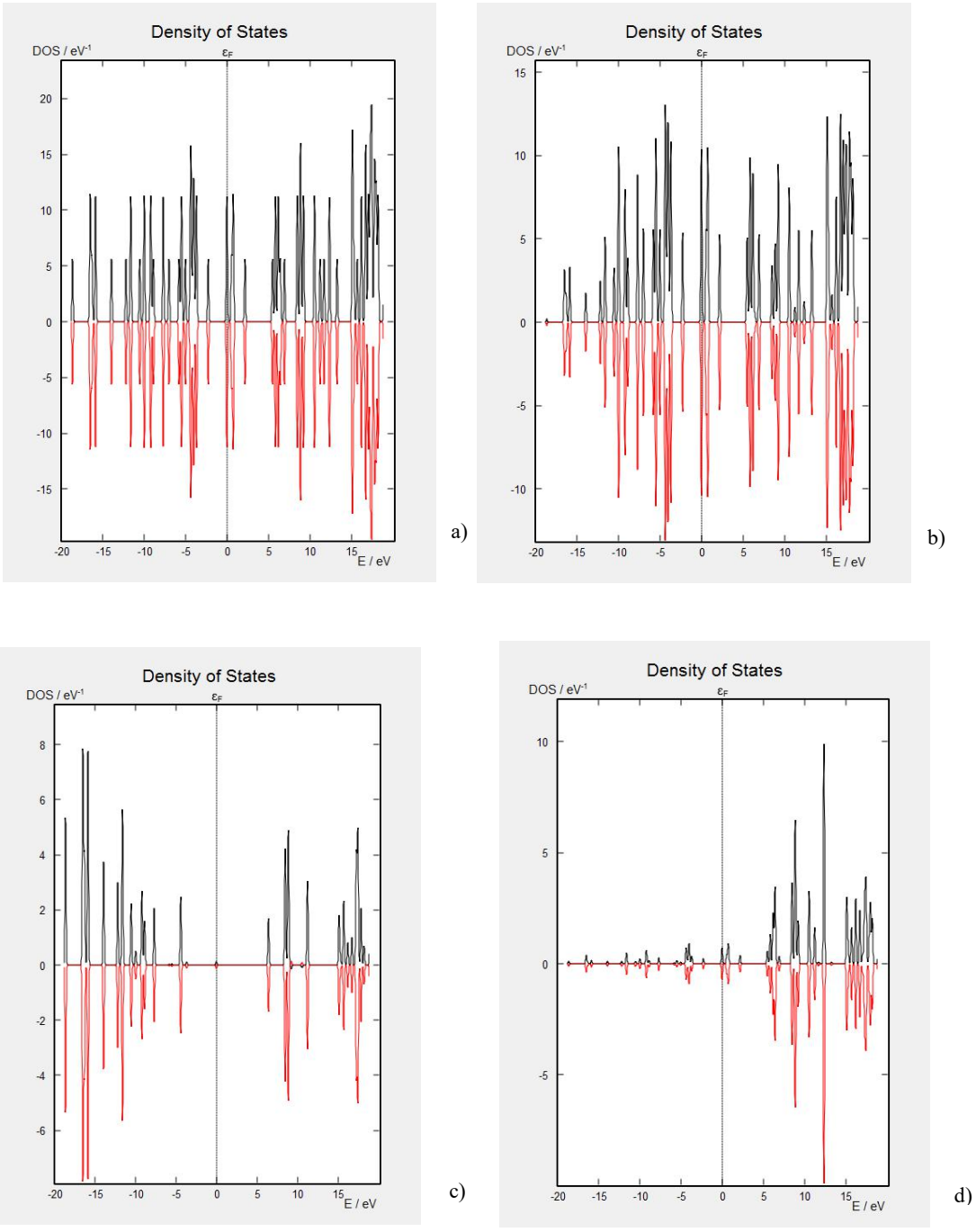
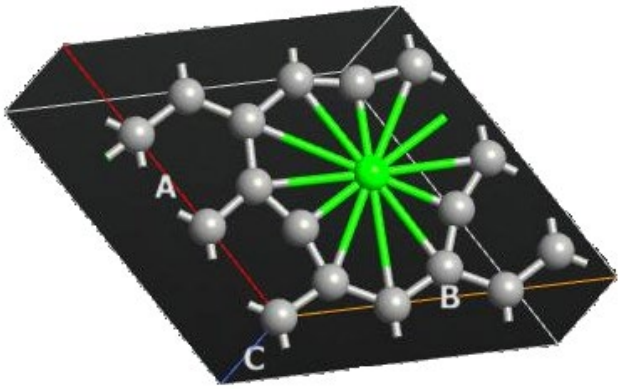


Fig. 1. The DOS for spin up and spin down p-, s-, d- electrons of the dopant Al atom in the 18 atom supercell: a) DOS, b) p-state, c) s-state, d) d-state.

Figure 2 illustrates the atomic structure of the Sr doped graphene plane and density of state.

In addition, this paper is devoted to investigation of magnetic properties of graphene doped with Sr (Fig. 2). In case of Sr atom substituted C 18 atoms in graphene calculated magnetic moment acquired 1,349μB. According to calculations, Sr (C) substitution leads to the ferromagnetic (FM) spin ordering.



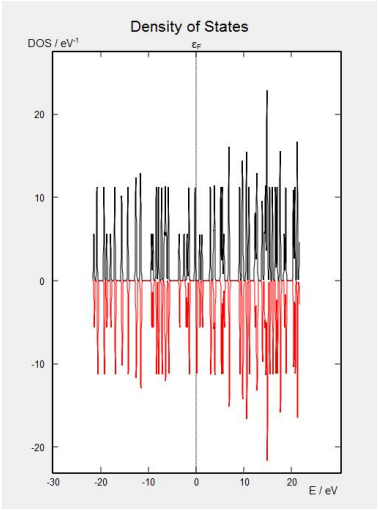


Fig. 2. Sr doped 18 atoms grapheme.

CONCLUSIONS

Ab initio calculated electronic and magnetic properties of Al, Co, Sr atoms doped graphene. To simulate the doping effect, we have introduced our calculations for 18 atom-contained supercells. In addition, our investigation demonstrated that Sr doping graphene is an effective route to obtain a magnetization. Total magnetic moment derived from Mulliken population analysis in the graphene by doping Sr is 1,349$\mu\beta$. In this paper has been also explored theoretically that in supercell constitute of 18 atom graphene carbon atom substitution with Al and Co this supecell appeared band gap 0.375eV, 0.76eV, respectively. Note that, we investigated density of state for graphene structure by the doping of Al, Co, Sr atoms.

According to providing theoretical program packet we are grateful to Guliyev Jeyhun programmer of the Institute of Physics.

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Received:27.10.2020