The Energy of Formation Hexagon-Shaped N-doped Clusters $C_{96-x}N_x$

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Several methods to eliminate some of the imperfection of grapheme – an infinite two-dimensional system of carbon atoms – are insisting. First it is, zero density single-electron states near the Fermi level, and second the lack of band gap. These included too the transition to a carbon nanoclusters (CNC) of finite size, creation of certain sets of mono- and polyatoms vacancies and doping graphene another atoms with an excess or deficiency of electrons in comparison with the carbon atom.

Presented here are the results of quantum-chemical calculations (DFT, B3LYP, 6-31 G**) clusters $C_{96-x}N_x$ (x = 1, 2) graphene-like structure.

Among the clusters $C_{95}N$ considered those, are obtained from the hexagonal C_{96} replacing one of the atoms C on atom N, consistently moving from the central hexagon to one of six zigzag edges. The most stable among them cluster with doubly coordinated nitrogen atom located in one of the zigzag edges with energy of formation, according to the model reaction $C_{96} + N \rightarrow C_{95}N + C$, - 79.8 kJ/mol for the electronic ground-state with multiplicity (M) is equal to four. Despite the rather substantial negative charge (0.38 a.u.) at the nitrogen atom, the spin density in the cluster is allocated in mainly doubly coordinated carbon atoms, as is the case in CNC C_{96} (M=5) [1]. For clusters $C_{95}N$ with various localization of nitrogen atom, the energy of formation is higher and negative charge on N is increasing according to moving the nitrogen atom from zigzag edges to the bulk of cluster, and reaching a maximum value in case when N located in the centre of hexagon. There are several vacant molecular orbitals (α- and β-) in monodoped clusters $C_{95}N$ with negative energy, indicating that transformation the CNC C_{96} (M = 5) into the *n*-type semiconductor with the energy difference between the highest occupied and the lowest unoccupied molecular orbitals ~ 2 eV.

Structural and energetic properties didoped clusters $C_{94}N_2$ (M=3) are largely dependent from the distance between the nitrogen atoms, *d(N-N)*. Thus, in case when one of N placed in the centre of hexagon and the other placed on zigzag edge, and is doublycoordinated, the distance *d(N-N)* is 7,47 Å. The energy of formation cluster $C_{94}N_2$ (M=3), according to a model reaction $C_{95}N$ (M=4) + N → $C_{94}N_2$ (M=3) + C, is already 413.2 kJ/mol. Due to the repulsion between nitrogen atoms (the charges in atom are - 1.08 and - 0.36) the energy of formation $C_{94}N_2$ (M=3) is increase in comparison with the energy of formation cluster $C_{95}N$ (M=4).

1. Karpenko O.S., Lobanov V.V., Kartel N.T. // Chem. Phys. Technol. Syrf. – 2013. – Vol. 4, 2. – P. 123.