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Interaction of fluorine with vacancies of graphene

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Chemical modification of graphene is a promising method aimed at changing its electronic properties and creating on its basis quantum structures. Fluorine, as hydrogen, is an element that converts graphene into a semiconductor material. One of the methods is the fluorination of graphene in aqueous solutions of hydrofluoric acid. The aim of the work was to study the interaction of F-, FHF- ions and their associates with water molecules with monovacancy and divacancy defects in graphene by quantum-chemical modeling. The C96H24 cluster modeling ordered graphene had a hexagonal shape with zigzag edges corresponding to the most stable configuration of the graphene sheet. Our model and approximation reproduce well the available literature data of the geometry and relative stability of monovacancies on a pure graphene surface, as well as fluorine adsorption on vacancies. As a result of the investigation, the energy characteristics of the chemisorption of fluorine from the associates of ions with water molecules were determined. It is shown that vacancies influence the chemisorption parameters: the activation energy decreases, the heat of adsorption increases in comparison with the ordered graphene sheet. The dependence of the heat of chemisorption on the degree of coverage by fluorine is studied. The characteristics of the reaction of vacancy defects with F-, FHF- and hydronium ion are compared. The results obtained can be useful for determining the optimum regimes for the synthesis of fluorographene with specified properties under laboratory conditions.

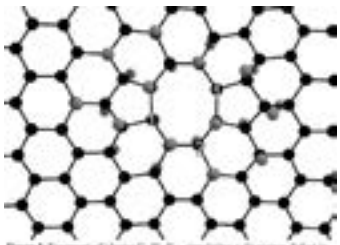

Figure 1: Fragment of cluster $C_{96}H_{24}F_{24}$ simulating a divacancy defect in graphene with 24 chemisorbed fluorine atoms. The most stable centers of adsorption are the marked atoms.

Recent Publications

1. Nebogatikova N A, Antonova I V, Prinz V Ya, et al. (2015) Fluorinated graphene dielectric films obtained from functionalized graphene suspension: preparation and properties. Phys. Chem. Chem. Phys. 17:13257-13266.
2. Lvova N A and Ananina O Yu (2015) Theoretical study of graphene functionalization by F- and FHF- ions from associates with water molecules. Comput. Mater. Sci. 101:287-292.
3. Lvova N A, Ananina O Yu and Ryazanova A I (2016) Fluorine and carbon fluoride interaction with a diamond surface: Quantum-chemical modeling. Comput. Mater. Sci. 124:30-36.
4. S Wang, X Ke, W Zhang, et al. (2014) Fluorine interaction with defects on graphite surface by a first-principles study. Appl. Surf. Sci. 292:488-493.
5. El-Barbary A A, Telling R H, Ewels C P, et al. (2003) Structure and energetics of the vacancy in graphite. Phys. Rev. B 68(14):1441071-7.

Biography

Annenkov Mikhail has completed his Graduation at Moscow Institute of Physics and Technology (MIPT), Russia in 2017. Currently, he is pursuing his PhD at MIPT. His research interest includes “Investigation of the diamond surface and two-dimensional structures by the quantum chemistry simulation”.

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