THE ADSORPTION OF HALOGEN AND HYDROGEN ATOMS ON GRAPHENE: THE NATURE OF BOND AND STABILITY

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Abstract

We studied bond properties of graphene's fluorinated derivatives and adsorption of fluorine, chlorine and hydrogen atom on graphene. For all calculations density functional theory was used. The character of C-F bond varies with fluorine concentration and local structure: one atom of fluorine makes ionic bond with graphene, but C-F in fluorographene (100% coverage) corresponds to a covalent bond. Configurations with fluorine atoms in trans positions are highly stable. On the other hand, hydrogen atom makes both noncovalent and covalent bond with graphene, which is weaker than a classical hydrogen-carbon covalent bond in other compounds. Chlorine does not make a typical chemical bond with graphene at all, but it creates a charge transfer complex. The strength of this bond is similar to the strength of the hydrogen-graphene covalent bond. Fluorine interacts more strongly with graphene than hydrogen and chlorine. Finally, adsorption of atoms significantly changes electronic properties of graphene.

Keywords: Graphene, fluorographene, adsorption on graphene, fluorinated derivatives, adsorption of fluorine, adsorption of chlorine, adsorption of hydrogen, density functional theory

Author did not supply full text of the paper.