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Stability and electronic structure of the functionalized graphene layers[1] JACEK A. MAJEWSKI, KAROLINA MILOWSKA, MAGDALENA BIROWSKA, MAGDALENA WOINSKA, University of Warsaw — We present results of extensive ab initio calculations in the framework of the density functional theory of the graphene layers (GLs) doped with nitrogen and boron, and also functionalized with simple OH, COOH, NH_n, and CH_n molecules. We calculate binding energies, heat of formation, resulting local deformations (characteristic sp^3 rehybridization of the bonds induced by fragments), electronic structure, elastic properties (Young's modulus and Poisson ratio), and conductance of doped and functionalized GLs as a function of the density of the functionalizing systems. Generally, the stability of the functionalized graphene layers decreases with the growing concentration of functionalizing molecules and we determine the critical density of the molecules that can be chemisorbed on the surface of GLs. We find out that the GLs functionalization leads in many cases to the opening of the graphene band gap and can be therefore utilized in graphene devices. In particular, the zero band gap in K-point of the pristine single GL increases to 0.11, 0.12, 0.25, and 0.24 eV for the GL functionalized with OH, NH, NH_2, and COOH, respectively.

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