Theoretical study of the influence of heteroatoms on the interaction of an aluminum cluster with a carbon graphene-like plane

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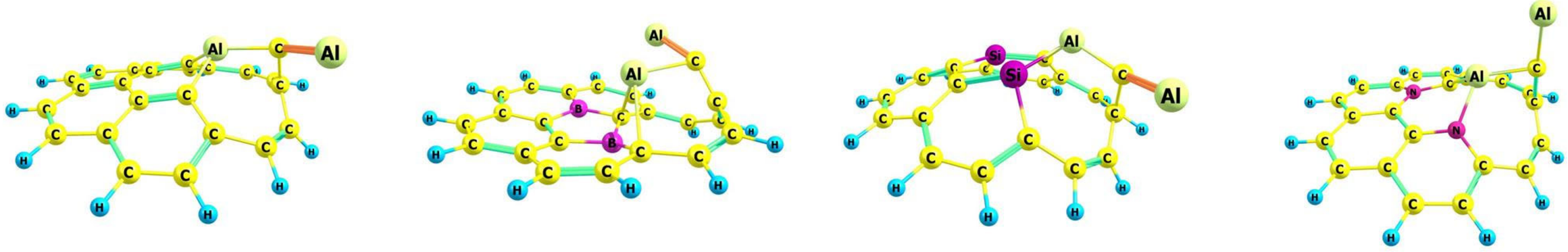
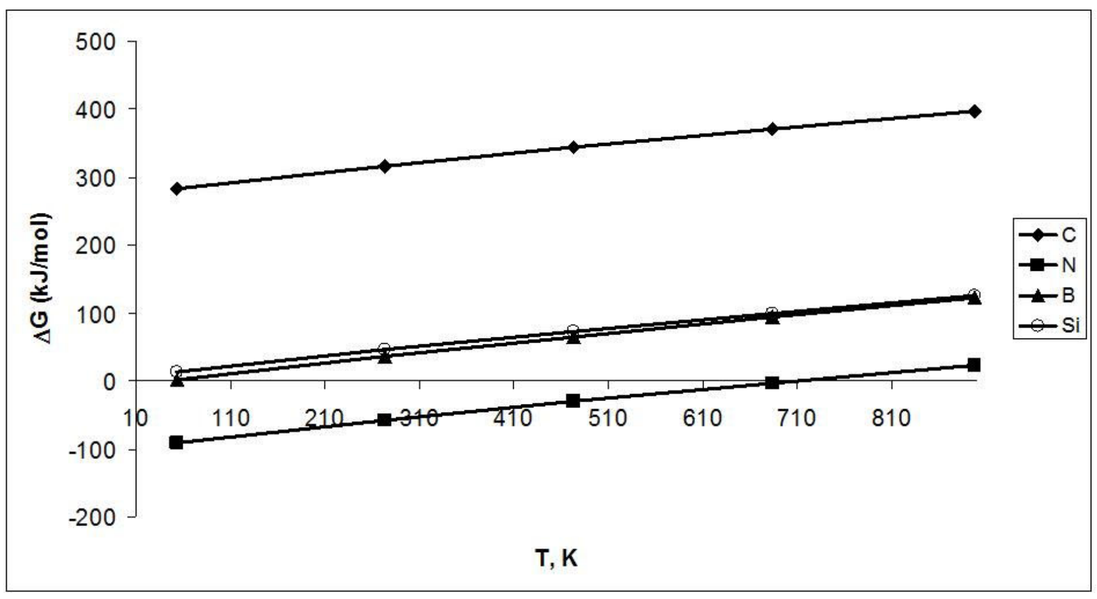
Today, one of the promising areas of modern science is nanotechnology [1]. It is important to obtain nanocomposites with a metal matrix, the creation of which is based on fundamental studies of physicochemical processes of formation of materials and their structure at the atomic level, which provides the possibility of obtaining nanocomposites with specified functional properties.

The aim of the study was to determine the effect of temperature on the chemical interaction of an aluminum cluster with native, boron-containing, silicon-containing and nitrogen-containing graphene-like planes. The calculations were carried out by density functional theory method with fuctional B3LYP and basis set 6-31G(d,p) by means of Firefly 8.2.0 program package.



Clusters of $C_{24}H_{12}$, $C_{22}B_2H_{12}$, $C_{22}Si_2H_{12}$ and $C_{22}N_2H_{12}$ were selected as graphene-like planes. The simulations were performed on the example of intermolecular complexes of a graphene-like cluster with a cluster consisting of two aluminum atoms that form a plane parallel to the graphene-like plane.



As a result of the interaction, aluminum atoms form chemical bonds with carbon atoms and graphene-like heteroatoms. In this case, one of the carbon atoms is located outside the conjugate aromatic system, which indicates the initial stage of destruction of this graphene-like plane with the formation of aluminum carbide.

. The results of the calculations show that the energy effect of the chemical interaction is for the native graphene-like plane +289.2 kJ/mol, for silicon-containing - +12.6 kJ/mol for the boron-containing plane, this value has a negative value of -2.4 kJ/mol, and for nitrogen-containing - this value is the lowest and is -100.4 kJ/mol. Thus, the presence of Nitrogen atoms in the formed nanocomposite aluminum-carbon matrix increases the energy of intermolecular interaction in the nanocomposite compared to the same value for the native, graphene-like plane, as well as with boron and silicon atoms.

1. Sheeparamatti B.G, Sheeparamatti R.B. Nanotechnology: Inspiration from Nature // IETE Technical Review. – 2007. – 24, N 1. – P. 5–8.