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CONTENT

COMPUTER-INTEGRATED MODEL OF AS-S ATOMIC CLUSTERS CONDENSATION

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For modeling with the use of first-principle quantum mechanical methods of condensation processes of four- and five-atomic As_nS_m clusters, it is sufficient to take a flat monolayer of the graphite structure with 12 carbon atoms the free valences of which are saturated with hydrogen as the smallest fragment of the carbon substrate. Theoretically, there have been investigated the condensation processes of 12 different clusters which are more stable in vapor phase and have different dimensional structure: chain, polygon, branched structure of a " star" shape, spatial shape of a "roof" type and closed polyhedron. For all such shapes of isomorphic forms of clusters the energies of their adsorption on the carbon substrate have been determined. For this, there has been used the value of full energy of the atomic system, consisting of a monolayer, substrate and the appropriate As_nS_m cluster optimally placed above its centre.

The analysis of modeling results shows that the adsorption on the carbon substrate of most As_nS_m clusters occurs due to the break of one or two of their chemical bonds followed by their transformation into the chain shape, which is covalently bonded with the substrate by its end atoms. Thus, the saturating hydrogen atoms of the substrate didn't form strong chemical bonds with atoms of clusters and had a little effect on energy and geometric parameters of their adsorption. Separate clusters with pentagon and polygon shapes are highly probable to be also adsorbed on the substrate without changes in their spatial shape due to Van der Waals forces (for As_4 molecules this is the main adsorption mechanism). In all cases the area of As_nS_m clusters during adsorption is positioned in parallel to the substrate surface.

The system achieves a deeper energy minimum if during adsorption not only the structure transformation of As_nS_m clusters occurs, but also the atomic structure of the carbon substrate changes, to a certain extent, especially on the edges and in the vicinity of those carbon atoms which are covalently bonded with the cluster. The most important of them are the change in their hybridization type from sp^2 to sp^3 by such atoms and their elevation above the surface of the graphite monolayer. Also, such changes have been substantially more significant if the covalent bonding of the cluster had occurred with the participation of more independent edge carbon atoms.

In most cases the value of adsorption energy of As_nS_m clusters on the carbon substrate can be approximately calculated based on the difference in energy levels of chemical bonds of the system before and after adsorption. However, such values are approximately~20 % higher than the values calculated with the use of the quantum-mechanical method DFT. Such differences are namely due to the forces of the mechanical tensions inside the system.