The Effect of Germanium Atom Adsorption on the Si (001) on its Density of Electronic States

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Different in the electronic properties of nanostructures and in the properties of bulk materials is caused by the presence of spatial quantization effects. The dependence of the band structure of an object from its size can be used for substantially increase the field of application of materials in electronic and optical circuits.

Nanostructures with germanium deposited on Si (001) are the most intensively studied among liked nanostructures and this has a number of objective reasons.

This paper presents the results of quantum-chemical calculations (method of density functional theory, B3LYP, 6-31G**) $Si_{96}H_{84}$•Ge nanostructures, modeling complex of germanium atom adsorption on the face of the Si (001). The energy its binding, of according to the results, was 7.8 eV. Thus there is a significant change in the density of electronic states both clusters representing the substrate and germanium atom. This change depends on the shift of the energy core-levels and valence electrons, so in an isolated atom Ge energy 1s core-level is 10,849.7 while this energy in the $Si_{96}H_{84}$•Ge cluster is 10850.94 eV. This energy shift is due, on the one hand, the displacement of the initial position of the core-level Ge atom at its entry into the modeling of the cluster, and the other - the electron relaxation subsystem original cluster representing of surface of the substrate. These changes can be negative and positive depending on increasing or decreasing the effective charge of the atom.

In addition to these factors to explain the shift direction is considered more Madelung potential - the total capacity, in this case an atom Ge, due to charges on the surrounding atoms. The relative contributions to the chemical shift of these factors are very difficult to individual of assessment.

Whereas Pauling electronegativity of Si and Ge atoms (1,8 and 1,7, respectively) can be explained by the positive shift level 1s Ge atom, assuming the dominant contribution of the first factor.

Core-level the 2s is shifted to 1340.3 (Ge atom) to 1340.9 eV are risen in the cluster, which also indicates the dominant role of the first factor.

Thus, taking into account the small absolute of values of the core-level shifts 1s and 2s atom Ge, it can be argued that the electronic structure of atom Ge undergoing minor changes in spite of the relatively high binding energy.