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Investigation of the population degree of atomic orbitals near impurity O and C atoms in the Si29H36 cluster

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The influence of oxygen and carbon on the electrophysical properties, characteristics and structural parameters of silicon is well studied. However, the cumulative effect of these impurities, especially with the noticeable influence of dimensional quantum phenomena during the transition to nano-scales, has not been sufficiently elucidated. This work is devoted to the study of changes in the population of electronic orbitals in the defect region and the effect of these changes on the main energy characteristics of the Si29H36 silicon nano-cluster containing impurity atoms O and C in volume using the computer simulation method.

To determine the contribution of an impurity defect to changes in the population of atomic orbitals and their effect on energy characteristics, the parameters of Si29H36, Si29COH36, Si28VOCH36 clusters were calculated using the ORCA4 software package [1].

Calculations performed to optimize the structural parameters and energy characteristics of Si29H36 and Si28OCH36 nano-particles by computer modeling showed a decrease in the symmetry group and simultaneous formation of Si-C and Si-O defects near the central T_d position (Table 1). In nano-particles, the formation of defects and changes in energy characteristics occur due to external, primarily radiation exposure. As the results of our calculations show, the formation of a vacancy does not yet lead to a decrease in symmetry, but due to population deviations around the local defect region, a global redistribution of covalent electrons occurs throughout the cluster and a partial transition to d-orbitals occurs in Si atoms. This ensures the stabilization of Si-O and Si-C bonds.

Thus, computer modeling and analysis of the results of calculations of the populations of atomic orbitals show that the simultaneous introduction of O and C atoms into the central coordination sphere of the Si29H36 cluster leads to the formation of defects with a decrease in symmetry, the stabilization of which occurs by the redistribution of electrons in the region of their formation. At the same time, the binding energies of R_{Si-O} and R_{Si-C} are greater than the binding energy of R_{O-C}, i.e. in this case, two types of defects are formed inside the cluster − Si-O and Si-C, although the electro-negativity of both O and C is greater than Si. The combined influence of the matrix atoms (i.e., Si atoms) and the effect of radiation leads to equilibrium with the redistribution of electrons involved in the formation of bonds and rearrangement of the electronic structure in the defective region.

Table.1. Energy parameters of Si29H36 nanoparticles and nano-particles formed by the introduction of impurity atoms O and C near the central T_d node.

nano-particle	Z_s	Z_d	E_g (eV)	nano-particle	Z_s	Z_d	E_g (eV)
$Si_{28}VH_{36}$	-	-	-4.7040	$Si_{29}H_{36}$	+	-	-5.1394
$Si_{28}VC_sH_{36}$	-	-	-3.5854	$Si_{28}C_sH_{36}$	-	-	-5.0552
$Si_{28}VOH_{36}$	-	-	-5.0214	$Si_{28}OH_{36}$	-	+	-3.0075
$Si_{28}VOCH_{36}$	-	+	-4.8250	$Si_{28}OCH_{36}$	-	-	-2.4277

Note: *C*s - atom C replaces 1-atom Si at the central T_d node; *Zs* - the charge of the surface of the nano-particle, *Zd* - the charge of the defect formation area inside the nano-particle, *Eg* - the width of the band gap.

REFERENCES

[1] Frank Neese. Software update: the ORCA program system, version 4.0, 17 July 2017.