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Nanosize Structures and Energy Parameters of Doped Silicon Clusters Passivated by Hydrogen

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The paper considers the computer model of silicon clusters doped with boron and phosphorus, and the effect of hydrogen on their structure and energy parameters. While calculating nanostructure formation, the model assumes hydrogenated Si_{29} clusters with substitution of a matrice atom with B and P impurities and insertion of one or some hydrogen atoms. Nanostructured defect complexes of Si-P-H or Si-B-H are suggested to be formed under hudrogen insertion, with their stability depending on the hydrogen atom number and the dopant type. Computer modelling and optimization calculations were carried out in the frame of nonempyrical modelling methods for structure and properties of multiparticle systems - ORCA under the approximation of local electron state density.

Keywords: Nanostructure, Nanosilicon, Doped, Boron, Phosphorus, DFT calculation.

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1. INTRODUCTION

Achieved success in nanotechnologies and nanomaterials and prospectives for their practical application stimulated theoretical and experimental researches of quantum mechanical and optical phenomena in nanostructures. The importance of studied of nanomaterials comes from the idea that almost any chemically stable structure can be obtained by proper manipulations with separate atoms or molecules. If the density of nanoscale structure at the interface is rather high, then the formation of such structures may result in crucial change of properties due to observation of quantum sized effects, such as quantum dots, wires and walls. In the case of semiconductors the structure of forming nanosized atom clusters corresponds to the quantum dots. The physical mechanisms of nanosized atom cluster formation and methods of their obtaining in semiconductors were reported in several papers [1-3] especially for silicon as the main material of semiconducting electronics and photovoltaics. It is known that formation of clusters of certain density in a crystal lattice results in changing of energy states of its components and significantly influences on the fundamental properties of semiconductor. The created systems with quantum dots represent a massif of nanoscale atomic clusters in a semiconductor matrix. Varying properly the sizes, shape and composition of quantum dots, one can obtain analogues of various natural elements. Really, used semiconducting matrices contain various doping impurities, which can significantly effect on formation of nanosized clusters and their electronical and optical properties. The main doping elements for silicon are Boron and Phosphorus as substitution impurities, which occupy the crystal lattice nodes. The formation of cluster nanostructures with B and P impurities was reported in several theoretical [1 – 3] and experimental [4, 5] publications, however there are contradictions in the obtained data. At the same time, it was proved experimentally [4] that technological growth and nanostructure formation proceed in the presence of impurity atoms and light gas molecules, like hydrogen, which can have a significant influence on the formation of nanostructures and significantly alter their atomic and electronic properties. Hydrogen is known as an active impurity both at neutralization of ruptured bonds on surfaces and formation of hydrogen containing defect complexes inside nanostructures. There is limited number of papers on doped quantum dots in Si involving hydrogen. For example, review [1] describes the study of electronic properties of hydrogenated Si quantum dots doped with one phosphorus atom by using the real space from the first principles and the pseudopotential method and the ionization energies and defect formation are calculated. However there are not enough theoretical and experimental works on spatial models of defect complexes in the doped silicon with hydrogen inside the forming low dimensional nanostructures [1, 5]. For predicting the effect of hydrogen on the properties of doped quantum dots, for example, for semiconducting nanocrystals, it is necessary to generate new and develop existing theoretical approaches to study of cluster structure models. The aim of this work was: to study the geometry, structure and energy characteristics of a silicon crystal fragment as nanostructure hydrogenized Si_{29} cluster, where the central atom is replaced with P or B impurity atom and one or a few hydrogen atoms are inserted nearby this impurity, and to build up a structure model of an optimized doped cluster.

2. METHOD FOR THE MODEL PARAMETER CALCULATIONS

To identify physical processes that take place with the formation of quantum dots and the effects of hydrogen atoms on them, it is necessary to accumulate data on the structural and energy parameters of silicon quantum dots with the involvement of different approaches. The existing theoretical calculations in sili-

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con nanocrystals are based mainly on two approaches: multiband method of effective mass with participation of electrons and holes, and the method of tight (strong) bond for modeling radiative and non-radiative processes in nanostructures. These methods take into account interactions of an inserted atom only with the nearest atoms of matrix, while the participation of accompany atoms or dopants in the nanocrystal formation and properties is not considered. Non-empirical theoretical calculations of physical parameters in the computer modeling of systems consisting of N_x particles assume the dynamical changing of electron gas in the field of slowly changing parameters of atom core. Since it is unreal to account all interactions between all electrons and atoms, in practice various approaches are usually implemented for simplifying the state equation, however the requirement of maximal possible reproduction of the structure and energy parameters of the real multi particle system must be kept unchanged. In this view the method of the density functional theory (DFT) is the most informative for description of the equilibrium energy state of electron structure and properties of interacting system of multi particles including atom clusters of semiconductors. The DFT method describes the total energy of cluster system with the formulae [9]

$$E_{DFT}[\rho]=T_S[\rho]+E_{ne}[\rho]+J[\rho]+E_{XC}[\rho] \,, \qquad (1)$$

where $T_S[\rho]$ – kinetics energy of all electrons; $E_{ne}[\rho]$ – energy of an electron attraction to a nucleus and $J[\rho]$ – energy of Coulomb repulsion of electrons in the system of mutually coupled particles; $E_{XC}[\rho]$ – energy functional for exchange-correlation interaction. All the functional are functions of electron state densities ρ. The exchange-correlation interaction energy is determined by

$$E_{XC}[\rho]=(T[\rho]-T_S[\rho])+(E_{ee}[\rho]-J[\rho]) \,, \qquad (2)$$

where $T[\rho]$ – kinetic energy of a particle system; $E_{ee}[\rho]$ – interaction energy of electrons involved in binding in the system. If a functional is found in the DFT method, then calculations are carried out analogously to wave mechanics: a set of orthogonal orbitals is determined by means of energy minimization. The advantage of the DFT method: it is necessary to calculate only the total electron density in the basic energy state of the interrelated particle system. If a functional is found in the DFT method, then calculations are carried out analogously to wave mechanics: a set of orthogonal orbitals is determined by means of energy minimization. The advantage of the DFT method: it is necessary to calculate only the total electron density in the basic energy state of the interrelated particle system. Therefore, we addressed to the well-known set of non-empirical methods for modeling of structure and properties of multi-particle system-ORCA (Optimization Rationalized Calculations Approximations by ab initio methods) in the approximation of local electron state density (DFT-LDA) (the 1-st order approximation to the density functional theory), where the electron state in homogeneity is taken into account [6]. The important aspect influencing the accuracy is the selection of a basic set of atom orbitals. If the choice is cor correct, optimization calculations will be done with the proper accuracy of both structure and energy parameters. We have used the basis set of atomic orbitals of the 6-31 G** for calculations, in which the polarization along all atoms is taken account and simulation of the core electrons is improved. The 6-31 G** is considered as the best compromise of speed and accuracy, and the most frequently used one by the basis set [7]. It is available for the elements from H to Kr. Then the non-polarized double exponent (DZ) set, of Slater type atomic basic functions (STOs) was used in the DFT approximated calculations by the BLYP method [8].

In this method, in addition to the full-electronic basis set, a set with the approximation of a frozen-core is also considered, which allows to increase the effciency of the calculation algorithms due to the decrease in the size of the basis. This approach makes it possible to apply the additional approximation *def*2/*J* to the theory of the density functional. The *def*2/*J* description is given in [9]. In the calculations of doped silicon clusters passivated by hydrogen, the following minimal basis sets for the Si are used: 16*s*10*p*1*d* which leads to 4*s*3*p*1*d* in the form of the {6631/631/1}; for the H, the 4*s*1*p* leading to 2*s*1*p* in the form of the {31/1}; for the P, the 16*s*10*p*1*d* leading to 4*s*3*p*1*d* in the form of the {6631/631/1}; for the *B*, the 10*s*4*p*1*d* which leads to 3*s*2*p*1*d* of the form of the {631/31/1}.

Moreover, the BLYP method involves the dependencies of exchange and correlation energy not only on the electron density but also on the density derivatives. Similar methods are known as Gradient correction techniques or Generalized Gradient Approximation (GGA). Most of them relate with functional modification LSDA (local spin density approximations). In the BLYP method the exchange-correlation energy with the gradient takes the following form

$$E_{XC}^{GGA}\left[n_\uparrow,n_\downarrow\right]=\int d\vec{r} f\left(n_\uparrow(\vec{r}),n_\downarrow(\vec{r}),\Delta n_\uparrow(\vec{r}),\Delta n_\downarrow(\vec{r})\right),(3)$$

where $n_\uparrow(\vec{r})$ and $n_\downarrow(\vec{r})$ – concentrations of electrons with spin-up and spin-down, respectively, $\Delta n_\uparrow(\vec{r})$ and $\Delta n_\downarrow(\vec{r})$ – their changes at interaction.

The exact analytical expression for the function $f\left(n_\uparrow(\vec{r}),n_\downarrow(\vec{r}),\Delta n_\uparrow(\vec{r}),\Delta n_\downarrow(\vec{r})\right)$ was derived in the integral form in [8]. But due to intricacy of the integral form application in the BLYP approximation, we used here the formula for the exchange-correlation potential obtained in [10]

$$V_{XC}\left[n(\vec{r})\right]=\frac{\partial E_{XC}[n]}{\partial n(\vec{r})}-\nabla\cdot\frac{\partial E_{XC}[n]}{\partial(\nabla n(\vec{r}))}, \qquad (4)$$

where $\frac{\partial E_{XC}[n]}{\partial n(\vec{r})}$ – partial derivative of the exchange-correlation energy term over a charge carrier density $n(\vec{r})$, $\nabla=\frac{\partial}{\partial r}$ – differential operator, $\frac{\partial E_{XC}[n]}{\partial(\nabla n(\vec{r}))}$ – partial derivative of the exchange-correlation energy term over a change rate of charge carrier density $n(\vec{r})$. Thus, for estimation the effect of exchange-correlation functional we chose the gradient-corrected functionals

(GGA) BLYP [7] and hybrid B3LYP (hybrid means a combination of exchange contributions determined by Hartree-Fock method and DFT-functionals) [9]. However, the use of the hybrid B3LYP method increases significantly the computer calculation time. In order to shorten the time, we used BLYP method for building computer models of clusters as had done before in [10] for studying effect of single impurity of phosphorus on structure and electron parameters of spherical diamond like hydrogen passivated $Si_{29}H_{36}$, $Si_{59}H_{60}$, $Si_{71}H_{60}$ nanoclusters with diameters of silicon cores 0.88 nm, 1.26 nm and 1.41 nm.

3. RESULTS AND DISCUSSION

Hydrogen passivated $Si_{29}H_{36}$, $Si_{28}PH_{36}$, $Si_{28}BH_{36}$ spherical clusters with very close sizes of silicon basis (0.86 nm, 0.84 nm, 0.88 nm, respectively) were chosen for calculation of impurity states of Phosphorus and Boron atoms, and also for studying the effect of hydrogen insertion on their properties in the silicon clusters. The diameters of clusters directly determined from the optimized coordinates, using the visualization by ChemOffice program. We assume that the central atom of the clusters are in the nodes of silicon single crystal lattice. For modeling of doped silicon single crystal, the optimized geometries of pure clusters were used, where one central silicon atom was replaced by Phosphorus or Boron, which was placed in the cluster center of the central coordination sphere. The effect of hydrogen insertion on the structure and state of such a cluster was considered not taking into account the way of insertion, i.e. from one to four hydrogen atoms placed nearby the central T_d position (tetrahedral symmetry point of diamond like crystal lattice of silicon). In general case, while cluster formation the system trends to the state with the minimal free energy, and in the most cases we deal with metastable clusters, which may have a significant temporal stability. Therefore, we chose those initial cluster structures, the optimization of which completed upon reaching the global minimum of the total binding energy. Modeling of substitution of Si atom in the central T_d position by impurity atom (P or B) was done only in such clusters, followed by modeling of insertion of one or some hydrogen atoms.

During hydrogenization, the cluster structure is stabilized and its diameter including the hydrogen shell does not exceed 1nm. The length of Si-H bonds on the surface is $R_{Si\text{-}H} \approx 0.15$ nm.

All the interatomic distances and average diameters of clusters were calculated for the optimized structures. Hydrogen induced structure changes were studied in dependence both on the number

of inserted hydrogen atoms and the impurity type in the cluster (see Fig. 1). The calculations of structures and energy characteristics of the clusters have shown[4] that small clusters undergo the maximal deformation: the impurity atom localized in the center of $Si_{29}H_{36}$ cluster results in distortion of the symmetry and the basis size growth. However the total cluster size increases slightly from 1.09 nm for $Si_{29}H_{36}$ to 1.15 nm for $Si_{28}BH4H_{36}$.

Inserting one H atom nearby P or B atom in $Si_{28}XH_{36}$ (X = P, B), T_d symmetry recovers completely, the volume slightly increases. The bond between inserted H atom and P or B is tighter than that between Si atoms in the 1-st coordination sphere. In the case of P impurity, the energy of hydrogen insertion is in good agreement with the chemical P-H bond (*length* ≈ 0.15 nm) in the defect Si-P-H complex. In the case of *B* impurity, the length of B-H bond ≈ 0.095 nm indicates the electron density increase around hydrogen containing defect Si-B-H complex. When inserting two H atoms nearby the central B atom, one H makes bond with B, another one bonds with Si on the 1-st coordination sphere, and the cluster core volume increases, while T_d symmetry persists. The inserted H atoms are placed symmetrically around B atom but do not make bonds. Two Si atoms of the 1-st coordination sphere make almost symmetrical bonds with P or B, and the 3-rd Si atom of the sphere does not make chemical bond with P atom, so the cluster core symmetry lowers from T_d to C_2. Insertion of three H atoms causes one P-H bond, and the rest two H are trapped by Si atoms of 1-coordination sphere, both the cluster core volume and symmetry persist. In case of B, insertion of three H atoms results in B-H bond, another H being close to B does not bond with it. And the third H makes bond with Si atom of 1-coordination sphere. Atom B slightly shifts from the central T_d position and bonds with two Si atoms of 1-coordination sphere that causes lowering of the cluster core symmetry to C_2. When at the beginning of the cluster structure optimization there appear simultaneously four H atoms around the central impurity atom (P or B) , while moving towards the equilibrium state, the symmetrical bonds are created (H-P-H or H-B-H) and the rest two H are trapped by Si atoms of 1-coordination sphere. Boron atom offsets from the central T_d position and makes bonds with two Si atoms of 1-coordination sphere. The symmetry of the cluster core lowers down C_2, the core volume increases and the distances between the surface Si atoms and the first neighbors of B atom are conserved. For the cluster with phosphorus impurity and inserted 2 or 4 H atoms, the P atom in the field of surrounding Si atoms is in 2-valent state, the rest two H atoms are trapped by Si atoms of 1-coordination sphere. But in this case these H atoms occupy anti-bonding states in accordance with the model suggested in [11]. For the doped clusters passivated by hydrogen, the width of the forbidden bands was calculated following way.

The energy level of the impurity electron is accepted as the top of valence band which is close to that of the Si <BH> cluster. As the bottom of the conduction band, the energy level of the impurity electron, which lies closest to the bottom of the conduction band of the Si <PH> cluster in the total count of the electron orbitals of the cluster, is accepted. The generalized formula for finding the width of the forbidden band for the doped hydrogen-clusters can be described by the following expression:

$$E_g = E_{HOMO} - E_{LUMO}\ , \tag{5}$$

where E_{HOMO} is the energy level, which lies closest to

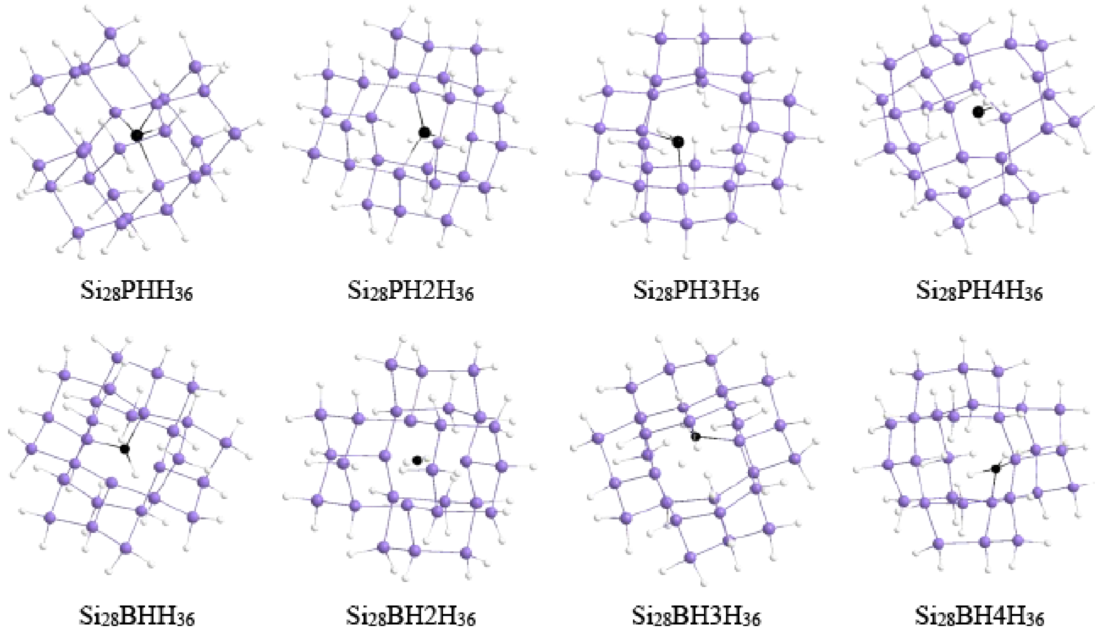

Fig. 1 – Change in the optimized geometry of cluster nuclei, depending on the number of inserted hydrogen atoms. Here substituting impurity atoms are labeled with black balls

the bottom of the conduction band of the cluster; E_{LUMO} is the highest lying energy level from the top of the cluster valence band. The calculated values of E_g are listed in the Table. Usually, the free energy change of a system at cluster formation with participation of impurity atom in the silicon crystal lattice can be expressed as [4, 5, 10].

$$\Delta E = -\Delta E_{\upsilon} + \Delta E_x + \Delta E_{ci}\,, \qquad (6)$$

where ΔE_{υ} – a free energy change resulted from transition of a system in more benefit energy state; ΔE_x – a free energy change caused by formation of a cluster surface; ΔE_{ci} – a free energy change due to elastic deformation of a cluster and its environment. The energy of formation of an impurity atom in a cluster is calculated by the following formula [8, 9]:

$$E_f = E(Si_{n-1}XH_m) - E(Si_nH_m) + \mu_{Si} - \mu_X\,, \qquad (7)$$

where $E(Si_{n-1}XH_m)$ is the total energy of a hydrogenized silicon cluster with an impurity atom; $E(Si_nH_m)$ is the total energy of a hydrogenized silicon cluster without an impurity atom; μ_{Si} is the total energy of a single silicon atom in a hydrogenized cluster; μ_X is the total energy of a single impurity atom in a hydrogenized cluster; For taking into ac-count inserted H atoms one more term should be added into formula 7, namely μ_H – the total energy of a single inserted hydrogen atom. The number of inserted hydrogen atoms is denoted as one. Then formula 7 will be as:

$$E_f = E(Si_{n-1}XH_lH_m) - E(Si_nH_m) + \mu_{Si} - \mu_X + l\,\mu_H \qquad (8)$$

The values of (see the table) for the modeled clusters with an impurity atom calculated by formulas (7 and 8) should differ significantly each from other because of bond formation in accordance with the exerted ambivalence of P: when one or two H atoms are inserted, surrounded by Si atoms P dopant behaves as two-valence ion forming quite tight P-H bonds. Impurity B atom, due to stronger B-H bonds than the P-H bond and a relative decrease in the electron density around this atom, has a higher kinetic energy The obtained results of calculations of optimal structures and characteristics in the framework of modeling the interaction of phosphorus and boron impurities with the hydrogen atoms inserted around them are in good agreement with those of [12]. The analysis of these calculations shows that phosphorus cannot hold more than two hydrogen atoms inside $Si_{28}PH_{36}$ cluster. Besides, independent on the number of inserted H atoms, at least one hydrogen atom remains electrically active. Unlike phosphorus, boron makes tight B-H bond with the inserted hydrogen, since all its valence electrons are involved in Si-B bonds, the hydrogen remains in the bonding state. It is true at inserting 2 H atoms, when the both B-H bonds are metastable and electrically active. But at inserting 3 H atoms one of them is trapped by Si and other two H atoms occupy non-active bonding and anti- bonding states. At inserting 4 H atoms around B atom, all of them are anti-bonding states. The calculated electron density in clusters, depending on their formation energy (Fig. 2), allows us to obtain the widths of the bands forbidden energy states (3rd column in the table) and to estimate the changes in the position of the energy level of the impurity atom, in the formation of defect complexes [P-Si-H], [B-Si-H].

In particular, for the impurities P and B, intruding of the hydrogen atoms leads to a change in the position of the electrically active impurity level in the forbidden

Table 1 – Changes of energy parameters at inserting hydrogen atoms around the central atom

Cluster types	Core diameter, Å	HOMO-LUMO energy gap, eV	Energy of formation of inserted H atoms, eV	Charges	
				The central atom	*H* atoms on the surface
$Si_{29}H_{36}$	8.81	3.86	–	– 0.07	0.01
$Si_{28}PH_{36}$	8.85	3.78	– 1.45(for replacing P atom)	0,04	– 0.03
$Si_{28}PHH_{36}$	8.81	3.02	– 2.91	– 0,40	– 0,04
$Si_{28}PH2H_{36}$	8.86	4.46	– 22.12	– 0,36	– 0,03
$Si_{28}PH3H_{36}$	9.18	3.82	– 19.33	– 0,36	– 0,03
$Si_{28}PH4H_{36}$	8.97	4.27	– 18,18	– 0,32	– 0,03
$Si_{28}BH_{36}$	8.78	3.82	– 1.5 (for replacing B atom)	– 0.78	– 0,03
$Si_{28}BHH_{36}$	8.56	3.17	28.61	– 0,79	– 0,03
$Si_{28}BH2H_{36}$	8.95	3.52	55.12	– 0,79	– 0,03
$Si_{28}BH3H_{36}$	8.91	3.21	5.56	– 0,69	– 0,03
$Si_{28}BH4H_{36}$	8.75	3,87	6,42	– 0,65	– 0,03

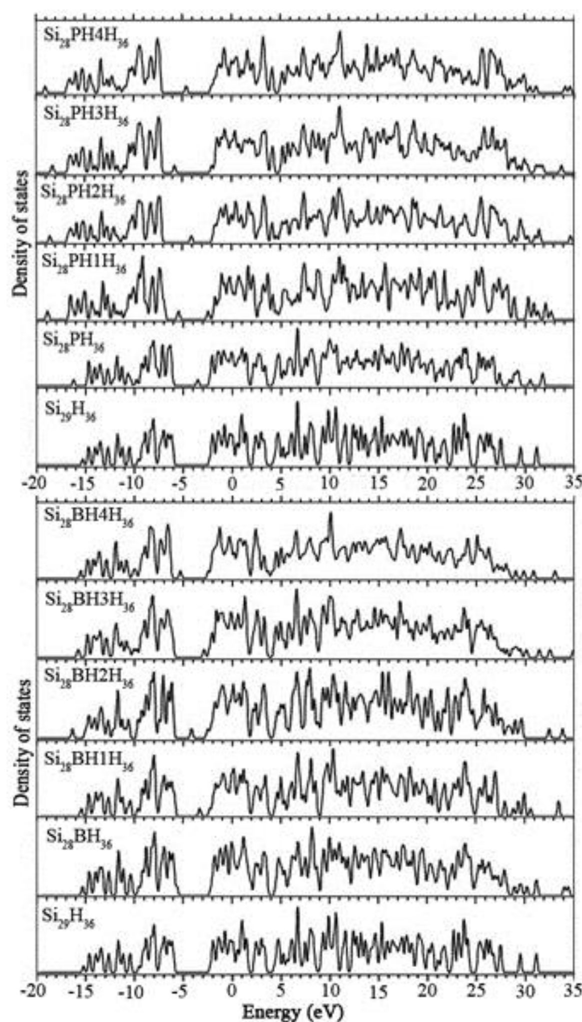

Fig. 2 – Dependence of the state densities in the $Si_{29}H_{36}$ cluster of doped P and B on the energy of their formation with a change in the number of intruded atoms hydrogen

band. Dependencies of the valence orbital occupancies in doped clusters were studied by us in [10], and in the models considered here we rely on our results obtained earlier at discussing the changes of the central atom charge and charges of surface. The results obtained here show that in the optimization process of the cluster structures, the hydrogen atoms inserted nearby the impurity atom of re-placement change significantly the charge distribution in-side the clusters. However, the chargeability of atoms on the surface change slightly (see the table) that is caused by the change of the coulomb radius of the defect complexes including hydrogen atoms (Si-P-H and Si-B-H) and by the charge redistribution around the impurity atom at inserting hydrogen. When the number of inserted H atoms increases, the symmetry of the cluster core structure lowers and the impurity atom displaces from T_d position and some of inserted H atoms are trapped by Si of the 1-st coordination sphere. It results in replacing of the defect complexes on the cluster subsurface coordination sphere and thereby changing of its forbidden gap.

4. CONCLUSION

Thus, at hydrogen atom inserting, the impurity phosphorus atom of substitution remains on the site, but the impurity boron atom is replaced on the subsurface coordination sphere and occupies a hexagonal interstitial position that results in lowering of cluster core symmetry from T_d down to C_2. Both the trapping of the inserted hydrogen atoms by silicon atoms of the 1-st coordination sphere and simultaneous forming of quite tight stable P-H (or B-H) bonds affect the stability of the structure energy state. Inside $Si_{28}PH_{36}$ and $Si_{28}BH_{36}$ clusters, the inserted H atoms may be in metastable electric active states. Inserting of single hydrogen atom in both impurity clusters causes the gap width increase. But a few inserted H atoms destroys the cluster core symmetry in the case of substituting phosphorus and boron atoms. Hydrogen atoms in antibonding state change the electron structure around the

impurity atom. As the consequence, the forbidden gap width gets quite sensitive to presence of more than one hydrogen atoms. It was shown that depending on the number of inserted H atoms the doped cluster size increases within the range of values: for boron impurity from 10.92 Å ($Si_{29}H_{36}$) to 11.49 Å ($Si_{28}BH4H_{36}$), and for phosphorus from 10.92 Å ($Si_{29}H_{36}$) to 11.31Å ($Si_{28}PH4H_{36}$) as compared with the clusters not passivated with hydrogen. It was suggested in the framework of considered models that at inserting one or two hydrogen atom the energetic stable defect Si-P-H or Si-B-H complex is formed.

While increasing the number o f inserted H atoms the defect Si-P-H complex persists, and the defect Si-B-H complex gets destroyed, followed by movement of impurity boron atom towards the cluster periphery.

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