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Optical Properties of the Semiconductor Nanoclusters

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Abstract. The paper presents the results of the study of the influence of external factors on the change in the morphology of nanoclusters in a matrix environment. Effective methods for calculating the optical characteristics of quantum-scale systems - semiconductor nanoclusters are highlighted. The prospect of combining theoretical methods of computer modeling (within the framework of molecular dynamics) with experimental studies of semiconductor nanoclusters in a matrix environment is illustrated.

Keywords: nanocluster, matrix environment, semiconductors, morphology, calculation methods, experiment

Actuality. Materials that contain nanoclusters have significantly different advantages. Varying the physicochemical characteristics of nanoclusters allows us to control the mechanical, electrical, and optical properties of a substance, in particular, a solid-state heterostructure **[1].** The presence of a nanocluster subsystem allows for more degrees of freedom for easy material reconstruction. Therefore, the study of the properties of nanoclusters expands the experimental limits and leads to the retention effect, increased mechanical stability and large surface area, and makes them suitable for photocatalytic activity**.** In particular, the luminescence observed in *por-Si* still arouses interest among specialists regarding the potential use of this material in optoelectronics [**2**]. One possible explanation is, in fact, quantum confinement caused by the formation of nanoclusters - nanometer-sized crystallites. The result is a partial violation of the rules of optical selection and the ability of the material to emit **[3, 4].**

Statement of the problem. The aim of the study is to analyze the influence of external factors on the change in the morphology of nanoclusters in a matrix medium. In this context, the main task was to identify effective methods for calculating the optical characteristics of semiconductor nanoclusters. In our opinion, an interesting prospect is the combination of theoretical methods of computer modeling (within the framework of molecular dynamics) with experimental studies of semiconductor nanoclusters in a matrix medium.

According to the set goal, the following **tasks** were solved: a) identify effective methods of computer modeling of semiconductor nanoclusters in a matrix medium; b) analyze studies aimed at determining the optical properties of nanoclusters in a matrix medium; c) highlight the specifics of experimental studies of semiconductor nanoclusters in a matrix medium.

Calculation procedure. To study atomic, electronic and phonon structures of nanoclusters, a method in the approximation of local electron density (LED) was proposed **[1].** Gradient decomposition is considered in the modelling. Several empirical parameters are applied in the proposed method. The use of a small number of parameters minimizes efforts in determining specific physical and chemical characteristics of nanoclusters. This approach is closely «linked» to the classic «ab initio» nanocluster research. It guarantees a good enough accuracy of calculations. As shown by comparison with the data submitted. The calculation scheme allows to study sufficiently large clusters (up to 100 atoms) with very good accuracy. In addition, the method allows to investigate the dynamics of processes within a standard molecular-dynamic procedure. The results we obtained indicate the possibility of joint consideration of real and model nanoclusters when conducting their test and functional diagnostics.

Optical properties of semiconductor nanoclusters in a matrix. The calculated molecular-dynamic analysis of polyhedral nanocluster systems of type $Z_{2n}\ H_{2n}$ (the symbol *Z* represents atoms of the 4 group Mendeleev's tab: *C, Si, Ge, Sn* and *H* is a hydrogen atom) shows that only certain spatial arrangements of atoms are possible in the nanocluster. The general trend of deformation energy behavior of polyhedral nanoclusters (PNC) depends on the number of quadrate rings (four-atom ring). The voltage decreases when four-atom ring becomes more. The energy of deformation for PNC three-five atoms ring is decreasing, although the number of four-atom ring in them increases. In addition, in these PNC s some angles between nanocluster in *n*-atom ring are close to the «ideal» values – $109,5^0$ (characteristic value for crystal semiconductor - *c-Si*). The energy of mechanical stress increases sharply with the subsequent increase in the number of atoms in the PNC, despite the increase in the number of four-atom ring. The reason for this behavior is the deviation of angles between chemical bonds in cyclic structures (120.0^0 for six - atom ring; 135.0^0 for eight - atom ring) in n-atoms ring from tetradimentric values («ideal» angles - 109.5^0). The lowest energy of deformation is characterized by PNC having a five-atom ring in the cross section. This conclusion confirms the possibility of experimental synthesis of a ten-atom PNC. To diagnose the difference in the nature of chemical connection between organic compounds and corresponding analogues of group IV, a concept of hybridization is proposed, which in this case acts as a unifying category. The higher analogues of IV groups have considerably worse possibilities for forming *s-p*-hybrid orbitals with a substantially higher p-type of communication, and therefore they retain the electronic configuration of types ns^2 and np^2. This is evidenced by our with different levels of approximation of small clusters with group IV atoms.

This behavior of these atoms is «convenient» for the existence of angles of $ca\text{-}90^0$ and formation of four-atomic rings with low mechanical stress. In contrast, the process of «formation» of trechatonic rings with angles 60^0 is impossible, since p-hybridization is the dominant method for defining «mixed» binding molecular orbitals. The above trend affects the relative stability of some Z_6H_6 isomers (where *Z=C, Si, Ge, Sn*).

It is well known that the benzyl ring represents a unique stable structure due to cyclically delocalized electrons. However, this stability is significantly changed if carbon atoms are replaced by group *IV* atoms.

Our calculations using mathematical model **[1]** of the distribution of electron density in clusters with *Z=Si, Ge, Sn* show that the hybridization of atomic orbitals is more active for forming double chemical bonds. As a result, the prism (with fully «passivated» chemical bonds) is more stable configuration than planar benzo-like clusters. The more stable isomers are those with less double chemical bonds. The increase of negative charge on atoms of a nanocluster frame reduces the difference in size between the angular s- and p-atomic orbitals, resulting in more hybrid atomic orbits. The energy *s-p* of promotion is reduced when the atoms on the carcass are concentrated with negative charge. Therefore, even in a treathoma ring with elements-type passivators SiH_3 are quite efficient «block» systems. Chemical bonds in small planar cyclic compounds are well oxidized, as the highest orbitals of silicon atoms are very strongly deformed. Therefore, the choice of substitutes is an essential factor in the process of successful experimental synthesis and separation of polyhedral silicon nanoclusters. The results of the simulation prove that a complete «protection» of atoms of cluster «skeleton» can be achieved with the help of bulky substitutes, which pass the attack from the external reagents. The efficient passivators in the process of synthesis are bulky quasi-rectorless configurations (matrix environment). We will describe them as groups in which halogen atoms are present. The spatial distribution of the passivating group determines the size and shape of the polyhedron. Structures with tetrahedral symmetry (tetrahedral symmetry group T_d) experimentally obtained by using reagents of type t-Bu_3Si. The latter play the role of the «defender» of atomic tetrahedron. X-ray crystallographic identification of Si_4Y_4 nanoclusters was performed for a larger structure where the packer function was performed by a $2(t\text{-}Bu_3Si)_4Si_4 \cdot (t\text{-}Bu_3Si)_2 \cdot C_6H_6$, recrystallizated group from a mixture Si_4Y_4 (here $Y= t\text{-}Bu_3Si$) with hexo-t-butyldilyane and C_6H_6 . The nanocluster has been found to be quite stable in relation to water, air and electromagnetic radiation (in visible optical range). The cluster «skeleton» has two different values of chemical $Si\text{-}Si$ bond length: $r(Si\text{-}Si) = 2{,}32\ A^0$, $r(Si\text{-}Si) =2{,}315\ A^0$, and β angle between chemical bonds is 59.9^0.

By using a gel-crystal-chromatograph in an active mixture of hexane and toluene, the specified polyhedral nanocluster structure (with germanium or silicon atoms) can be isolated in an organic matrix environment as a yellow or orange crystal at temperatures above 220^0 C . This atomic framework is quite photosensitive structure, despite its organic environment. In solid state, the crystal containing a marked nanocluster polyhedral fragment is thermally stable and does not change its properties within several months of its presence in the atmosphere.

Model analysis of the PNC Si_6Y_6 (D_{3h}) in a matrix environment (with the use of inter-interaction potentials and our model approach, allows to detect small distortions of prismatic structures. The prismatic polyhedral quartz of silicon or germanium is characterized by an absorption spectrum ranging from yellow to orange **[5].** Ultraviolet radiation detected for: 1) Si_6Y_6 - polyhedra, where matrix is $Y=2,6\text{-}i\text{-}Pr_2C_6H_3$ (*241 nm*); 2) Ge_6Y_6 a polyhedron, where matrix is $Y=2,6\text{-}i\text{-}Pr_2C_6H_3$ (*261 nm*). It should be noted that the «tail» of the absorption spectrum will be pulled into the visible region (500 nm). High photoresist sensitivity of polyhedral nanoclusters can be explained by the fact that under the action of radiation (with wavelength *340-380 nm*) at low temperatures new absorption bands are generated (*335 nm, 435 nm, 500 nm*) and under the influence of light excitation on six-atomic polyhedral nanocluster with a wavelength λ, more than *460 nm*, these bands are instantly regenerated **[1,6] (Fig.1).** The described PNC compound is thermally stable in a matrix environment at low temperatures (-150°C) which has a smooth return to the prismatic configuration **[7]**.

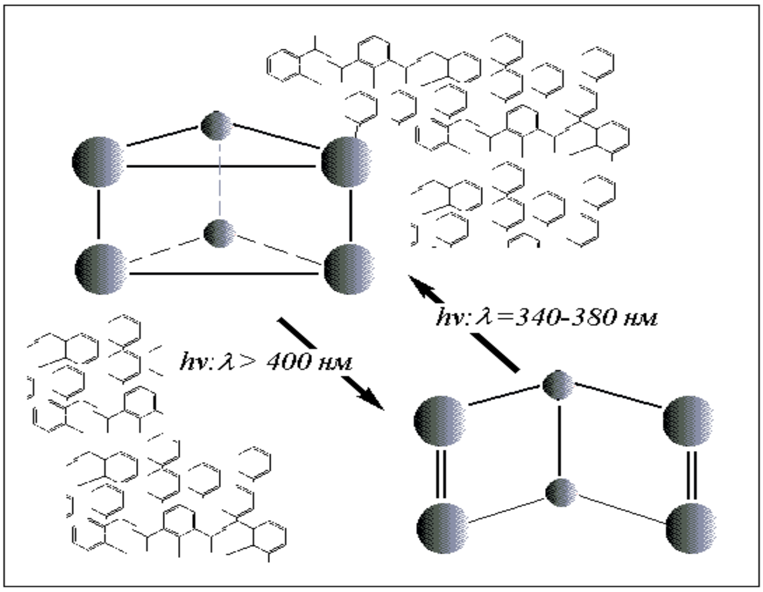

Fig. 1. Diagram illustrating possible chemical connections of polyhedral nanostructure

We estimate that the activation energy of this transition corresponds to the magnitude of eV. This is probably due to the disappearance of one quadrangular ring and the formation of double chemical bonds by crossing. This small value of chemical link switching energy indicates the high activity of double (*Si-Si*) chemical link. Due to the small forbidden zone of the prismatic cluster, the thermal reaction above the chemical bond transition is a formally forbidden effect. The interaction of *Si-Si* chemical bonds causes the splitting of molecular orbitals: on binding and antibonding orbitals. The transitions between the electron levels and meet an experimentally determined absorption band with wavelengths *455 nm* and *335 nm*, respectively. The lowest energy of transition corresponds to the width of the forbidden zone. The weak absorption line for *550 nm*.

Nanocluster structure, which is «built» from an eight-atom polyhedron (Si_8Y_8 (O_h)), according to experimental data, can be synthesized in a chemical condensation process channeled by alkaline metals in tolole [**7**] in the form of a bright yellow crystal with cubic symmetry. The role of the matrix, i.e. environment, is played by compounds: 1) Y=*t-Bu*; $Y=CMe_2CHMe_2$ or 2) Y=*Br*; Y=*t*-$BuMe_2Si$. Under the action of various chemical additives, allowing to vary type of substitutors, crystal can become different color: purple, red-orange, orange. The X-ray flow analysis allows to determine the average distance between the silicon atoms in an octagonal polyhedral structure (Si_8Y_8) ($2,384A^0$ - $2,411A^0$), as well as the mean value of the angle between *Si-Si* chemical bonds ($88,9^0$-$91,1^0$). The nanoclusters Si_8Y_8 we calculated retained their fairly high symmetry, unlike the structure found experimentally in the crystal. The reason, apparently, is that the bulky substituting-packers around the atomic framework play a spatial «defender» role, since the energy losses on conformational transformations of the polyhedron are significantly smaller. Experiments show that the kinetics of nanoclusters depend on the spatial-geometric characteristics of substituting-loaders, which play a role of matrix environment of cluster frame.

A striking feature of semiconductor nanoclusters is the dependence of their optical properties on the geometric arrangement of the atoms that form the nanocluster and its size. When the size (or geometry) of the nanoclusters changes, the energy state of the electrons also changes, and the oscillator strength is concentrated on only a few transitions. Such quantum limitations arise as a result of changes in the density of electronic states. According to quantum theory, for a free particle or a particle in a periodic potential of a solid, the energy and momentum of the crystal can be precisely determined, while the position of the particle cannot be determined uniquely. For a localized particle, the energy can still be precisely determined, but the uncertainty in the position is reduced, so that the momentum is not precisely determined**.**

Experiments show that these prisms have absorption in the visible region. Si_6H_6 has an absorption band with a maximum at 241 *nm*, which ends to *ca* 500 *nm*. The absorption band of Ge_6Y_6 (Y=2,6-*i*-$Pr_2C_6H_3$) has a maximum at 261 *nm*, which is red-shifted compared to Ge_6Y_6 due to the higher-lying *Ge-Ge* bond orbitals. In particular, the kinetic stability of tetrasilatetrahedrane (Si_4H_4), hexasilaprismane (Si_6H_6) and octasilacubane (Si_8H_8) depends significantly on the stoichiometric volume of the matrix passivators. Silyl-substituted Si_nY_m (Y= *t-Bu*) is stable in an inert atmosphere. But it oxidizes well in air, forming colorless solids. 1,1,2-trimethylpropyl-substituted Si_nY_m ($Y=CMe_2CHMe_2$) is extremely stable, even in air, and is preserved for two weeks in the solid state. Prisms with *Si* and *Ge* skeletons are yellow to orange in color [**6,8**].

The results obtained by us of calculations of polyhedral silicon nanoclusters allowed to determine not only the degree of planarity, but also show that when moving from element to element (*Pb-Sn-Ge-Si-C*) there is a decrease in the delocalization of electronic density in the cyclic structure. We have diagnosed the manifestations of individual-characteristic properties of atoms that form nanoclusters. These atoms determine the reactive capacity and kinetic stability of nanoclusters. The relatively high stability of pyramidal nanoclusters is due to the presence of electronic effects, which are characteristic only for silicon. We have functionally defined the role of substitutes, forming matrix environment of nanoclusters **[9].** The influence of passivators on the properties of nanoclusters is so significant that it can affect the change in optical properties of the system, energy stability and therefore the stability of the devices created on their basis. The passivity of silicon atoms to form multi- (double, triple) chemical bonds was shown; significant influence of the degree of polyvalence of inter-atomic chemical bonds in the process of stabilization of nanoclusters. It is shown that the stability of nanoclusters increases inversely in proportion to the number of double bonds. Optimization of the geometry of polyhedral nanoclusters allows to demonstrate the influence of substituents on the redistribution of electron density in different isomer structures.

We will analyze medium-sized polyhedral nanoclusters. Geometric and energetic analysis of tetra-, penta- and hexoplanar nanoclusters indicates that the increase in the angles between chemical bonds in the n-atomic rings is caused by an increase in strain. Thus, for $Si_{20}H_{20}$ nanocluster, changing the valence angle for the ideal tetrahedral configuration of 109.5^0 to a value of 144^0 causes an increase in the strain energy of the nanoclusters by the value *10,94 eV*. We emphasize that for $C_{20}H_{20}$-nanocluster the value of strain energy is much larger (*21,36 eV*). $Si_{20}H_{20}$ nanocluster exists in three isomeric spatial configurations: prism, pagodahedron and dodecahedron (**Fig.2**). The nanoclusters shown in Fig. 2, b, c are less deformed structures and thus more stable than the prism-like nanocluster. I_h is a cage structure (dodecahedron) formed by a skeleton of silicon atoms connected by chemical bonds, the angle between which is close to tetrahedral.

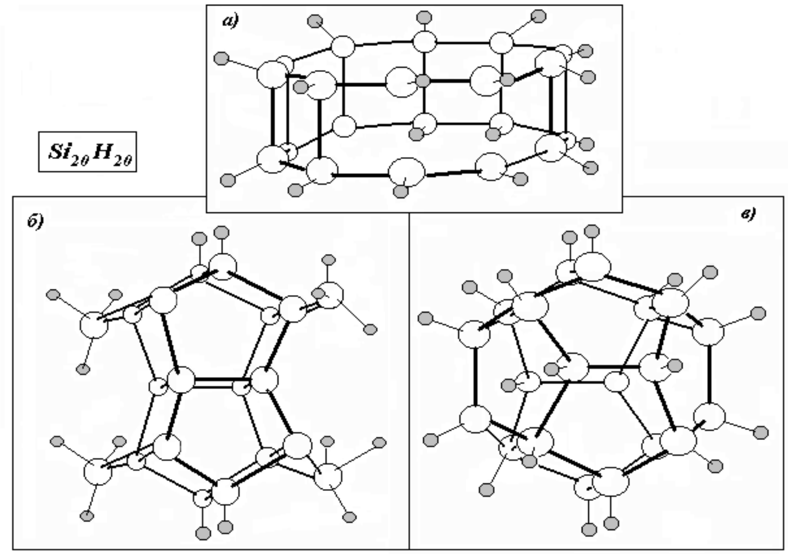

Fig. 2. $Si_{20}H_{20}$ nanocluster isomers: a-prism, b-pagodan, c-dodecahedron

Experimental analysis of the distribution of cluster ions with six (Si_6) and ten (Si_{10}) silicon atoms in the gas phase suggests that small-sized nanoclusters form isomeric Si_{60}-nanostructures. Two Si_{60}-nanoisomers that are described by symmetry D_{2h} and C_{2V} have a similar to cylindrical (i.e. elongated) shape. Our calculations show that the nanocluster in and modifications have quite high strain energy. This fact confirms that the process of gas-phase fragmentation of Si_{60} nanoclusters is not simple, but goes through a series of metastable transformations. In the cross section, a Si_{60} nanocluster with D_{2h} symmetry has two six-atom rings and C_{2V} symmetry has one ring.

The joining of planar five-atom rings is an energetically unfavorable process because the strain stress of Si_{60} nanocluster increases. If the number of neighboring penta-atomic rings increases and the number of six-atomic rings remains constant, the spherical-like nanostructure of 60 silicon atoms becomes smaller in size. Moreover, its stability decreases. This is confirmed by corresponding calculations: Si_{60} nanocluster with I_h symmetry is more stable than spheroidal nanostructures. In the larger spheroidal nanoclusters (Si_{70}, Si_{78}, Si_{84}) the number of planar six-atom rings increases.

The thermodynamic stability of these systems is not much higher than that of Si_{60} nanocluster. Complete passivation of the broken bonds by hydrogen atoms of Si_{60} nanocluster leads to the formation of nanostructure $Si_{60}\,H_{60}$. Geometry optimization based on molecular dynamic calculation shows that the optimal spatial arrangement of atoms in $Si_{60}H_{60}$. nanocluster should correspond to I_h symmetry (and possibly lower). Taking into account the effects of electron correlation leads to an insignificant change in the energy characteristics of such nanoclusters.

We denote the «diameter» of the empty cage sphere (nanocluster with I_h symmetry) by the symbol d. According to our estimates, this value for the fullerene nanocluster C_{60} is $7.1\ A^0$, and for the sphere-like nanostructure Si_{60} this size is larger by almost 54-60 %%, and corresponds to a value in the range from $11.1\ A^0$ to $12.3\ A^0$. One of the noteworthy properties of spheroidal nanoclusters is the ability of these configurations to encapsulate an atom, ion, molecule or small nanocluster fragment. These are the so-called endohedral complexes. Si_{60} nanocluster with I_h symmetry is more polarizable compared to fuleren C_{60}. Therefore, the formation of endohedral spherical nanocomplexes seems to be possible with significant atom and ion sizes. In the process of diagnostics of polyhedral nanoclusters it was found out that the charge transfer from encapsulated ion (or atom) to the periphery of spherical-like «cell» of Y_{60} (Y=C, Si, Ge) type (and vice versa) is an unlikely process. The nature of the interaction in the nanocluster spheroidal complex is electrostatic and causes polarization. In this case, the radius of ions inside the I_h nanocluster increases significantly compared to their isolated state. This is especially evident in large Si_{60} and Ge_{60} systems.

Having analysed the experiments we can note a clearly identifiable cluster raster. Silicon nanoclusters form an «island» structure on the semiconductor surface. In the micrograph, which is shown in **Fig.3**, the silicon nanoclusters are shaded by carbon atoms. Here, the degree of dispersion of silicon nanoclusters with sizes between 15 and 20 A^0 is of particular importance. Such a clustered silicon surface (at 100°C) with a metal-cluster raster of subcolloidal dispersion, with individual nanoclusters less than 15 A^0 in size, can be used to produce a spectrally-invertible photovoltaic cell**.**

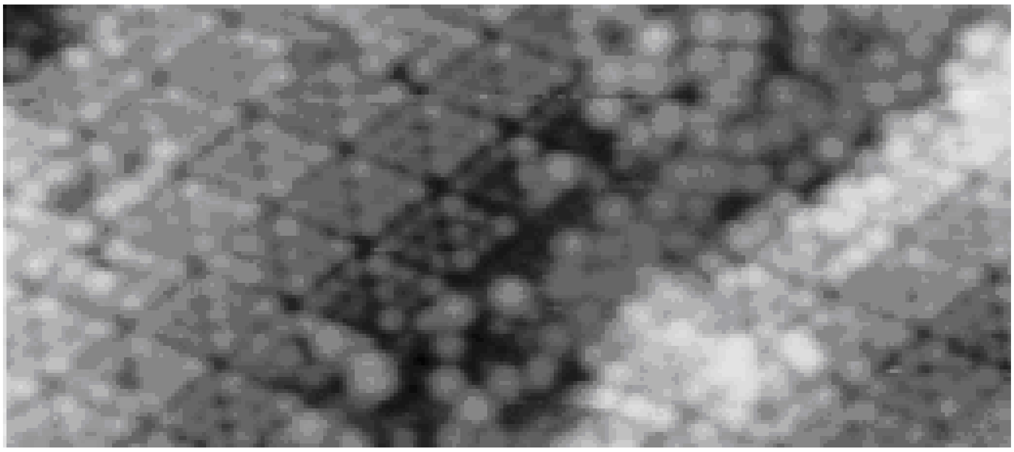

Fig. 3. Micrograph of nanocluster raster on silicon surface **(ref.[10]) .**

In addition, the effects of ‘encapsulating’ atoms, ions or even molecules inside a caged nanocluster structure with a sufficiently large number of atoms are very promising: 60 or more. The encapsulation of cations inside the cage-like I_h structure (C_{60}, Si_{60}, Ge_{60}) allows actually preserving the typical orbital symmetry of the neutral Y_{60} configuration. In this case, both energy limits (E_c and E_V) are stabilized (fixed) by «encapsulated» cations (X^+), resulting in an increase in the ionization potential and electron affinity for Y_{60} nanoclusters. For silicon nanoclusters with encapsulated cation, the forbidden band width decreases weakly. For caged nanostructures with carbon and germanium (our estimates), this energy band does not change. If we replace the cation with an anion, the situation is dramatically reversed. The limiting molecular orbitals are significantly destabilized. The electronegativity increases and tends to the electron affinity of the polyhedral structure.

Comparing the behavior of anions and cations (within our computational approach) within a cage type structure allows us to characterize the concept of so-called hard and soft interactions. For silicon and germanium nanocluster, cations perform the stabilizing role more effectively, while anions destabilize these polyhedra. In carbon fullerenes, the geometrical configuration is stabilized by all ions except for the “large halogens” (Rb^+, Br^-, I^-), whose radius is commensurate with the radius of the cage nanostructure, which can lead to spatial destabilization of the endohedral complex.

The discrete energy eigen functions of the particle may then be viewed as super positions of bulk momentum states. Given the relation between energy and momentum in the bulk solid, one can see how a series of nearby transitions occurring at slightly different energies in the bulk be compressed by quantum confinement into a single, intense transition in a quantum dots - nanoclusters. Polyhedral nanoclusters, which are characterized by the symmetry group O_h, can be used in modelling the optical properties of porous silicon (*por-Si*).

Por-Si and polyhedra nanocluster have the same influence on the width of the photoluminescence spectrum, and on the large Stox shift. The chemical shift of polyhedral varied in the range {from -22 to 39} *ppm*. Experimental studies Si^{29} - NMR of the spectra, show that the deformation of atomic polyhedron type Si_8Y_8 with $Y{=}t\text{-}BuMe_2Si$ is anisotropic.

Luminescence energies on porous silicon or silicon nanocrystals. The research results show that the luminescence of samples of porous silicon is subject to large red shift when exposed to air and with an average size of nanoclusters less than *3 nm*. Luminescence measurements on silicon crystals obtained by decomposition of silane agree well with the theory. However, luminescence is observed only for fairly large crystallites. Thus, the situation is complex, even if the oxidation state of the samples seems to play an important role in the recombination mechanisms.

All these results suggest that other channels for the radiative recombination are possible. Large Stokes shifts might be consistent with the eventual existence of deep luminescent centers. The problem is that nothing is presently known regarding the nature and origin of these states. Our calculations that such states indeed exist under the form of self-trapped excitons, most probably at the surface. A possible situation is the trapping of an exciton on a Si-Si bond of a surface dimer whose dangling bonds are saturated by hydrogen atoms.

We find another interesting situation with very small crystals containing less than 50 silicon atoms. We systematically obtain a large atomic relaxation in the excited state, which causes an important reorganization of the bonds in the nanocluster. The consequence is a large Stokes shift between absorption and emission energies. Thus, the nanoclusters, whose optical properties have been described above, may play an important role in the luminescence of porous silicon.

In addition, Si_xGe_{1-x} alloys are characterized by improved optical properties compared to pure silicon. Therefore, such materials are very promising. Using the parameterized density functional method described in **[1,8],** we investigated the confinement effects in *SiGe* nanoclusters. Sphere-like nanoclusters passivated by a hydrogen atom were considered. Atomic positions were randomly occupied by Si or Ge atoms. Our results show that the band gaps of nanoclusters such as $Si_{0,8}Ge_{0,2}$ and *Si* are quite close and comparable with a blue shift. This is due to the fact that the electronic states in bulk *SiGe* alloys are still delocalized. That is why they experience the full confinement effect as in crystalline silicon (*c-Si*).

We now analyze the case of stronger disorder as obtained in amorphous silicon (*a-Si*). It raises extremely interesting problems related to the confinement induced blue shift of the energy gap: (a) does it exist in clusters of a-Si and is it comparable to what is obtained for *c-Si*; (b) what is the behavior of disorder-induced localized states in this regard. It has been often assumed that quantum confinements effects are small in *a-Si* nanostructures due to the short coherence length of free carriers in these materials. We will see that it is not true.

Conclusion. Thus, we have discussed in detail the optical properties of silicon nanoclusters in a matrix medium. Our studies confirm the high efficiency of the parameterized method used to study the optical properties of these objects. Comparison of theory with experiment shows the possibility of the existence of various radiative channels for recombination in porous silicon, which is a complex material.

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