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NANOELECTRONIC'S MATERIAL FOR OPTIC SYSTEM

The theoretical approach of quantum-dimensional system we have discussed. Our results are important for visualization and generation nanodimensional parts of the optical system.

An semiconductor surface is specific surface disordered phase (SDP) and the main peculiarities of modern nanoelectronic devices depend on the individual parameters of the surface phase. Furthermore, the reactions of atomic hydrogen (H), fluorine (F), chlorine (Cl) and bromine (Br) with Si surface were widely studied experimentally and many investigators have observed the semiconductor SDP directly [**1-3**]. For a quantitative analyses of nanostructures like nanoclusters (NC) creation in Si and other solid materials the clusters distribution along the surface is necessary.

On the other hand, the recent progress in the combination of visualization with simulation techniques have concurred to obtain spectacular results in the investigation of chemical reaction mechanisms as well [**4**]. The traditional quantum chemical ab initio methods, based on the Hartree-Fock scheme have become well established in studies of the electronic and geometrical structure of the solid NC [**1**]. Therefore, the surface NC as real objects and model in the nanoelectronic's material for intelectual system is great interest.

Our Model Molecular Graphics Package (MMGP) which is specially designed so as to allow for high-level computerized visualization in molecular science. MMGP contains many interfaces with quantum chemical programs such as the semiempirical and molecular surface geometry generation, which is based on the interatomic potential (for example, Modified Stillinger-Weber (MSW)).

In the paper development and applications of the MMGP to the Si-NC was demonstrated. The MMGP generates detailed and easily interpretable and aesthetically appealing graphics representing models of molecular structures and related properties. The package offers a high level of interactivity through the use of the mouse and via a large set of menus and submenu, organized in such a way so as to enable users to learn rapidly the basic operations leading to efficient visualization (see **Fig 1,2.**).

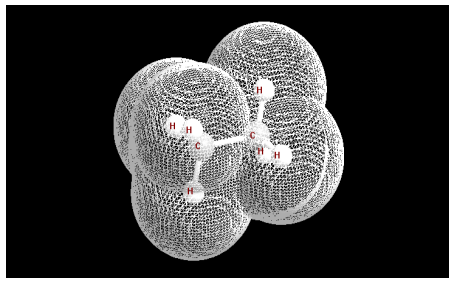

Fig 1.
Map of the density electron distribution for the nanocluster

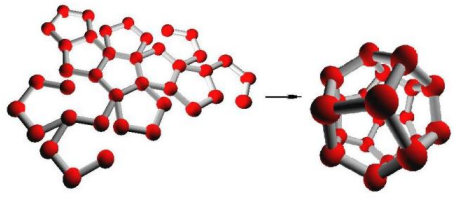

Fig.2.
3D-representation of the
nanoparticle's formation from nanocluster

For all the menu items, a help facility has been implemented. Various representation options and attributes may be selected for adapting the visual output to personal needs and preferences:

the molecular structures may be represented as discrete dots, and the global appearance may be modified via attributeS such as back ground appearance, perspective or orthogonal projection and others. The purpose of the MMGP is the interactive visual representation of three-dimensional (3D) models of molecular structures and properties for research. Due to the flexibility of the data- and program-structure, various chemical systems ranging from small compounds (clusters) to large macromolecules may be investigated; additional interfaces and tools can easily be implemented. The MMGP contains the tools which are neccessary for the investigation and visualization of the results generated by the calculation program-package contains:

- Modified IEHT-α method.

This is for semiempirical calculations of one-electron level energies, wave functions and other parameters of electronic structure of NC. The estimation of the total energy of clusters which has different size is follows:

$$E_{tot} = \sum_{A \neq B} \frac{Q_A(\vec{r}_{AB}) - Q_A^*(\vec{r}_{AB})}{r_{AB}} + \\ + \sum_i g_i E_i - (E_{ee} + E_{exc}) \quad (1)$$

$$E_{exc} = \sum_{A \neq B,}^{all} \sum_{\mu \neq \nu}^{occ} \frac{1}{r_{AB}} \nu_{AB} S_{\mu\nu}^2 \quad (2)$$

υ_{AB} is the fitting parameter.

→POTENTIAL package.

This is simulation programme for calculations based on different types of interaction potentials. One of them is modified Stillinger-Weber-type potential [2]. Hamiltonian is follows:

$$H(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_N, \vec{p}_1, \vec{p}_2 \ldots \vec{p}_N) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \\ + \sum_{i<j}^{N} V_{\text{int}}^{(2)}(\vec{r}_{ij}) + \sum_{i<j<k}^{N} V_{\text{int}}^{(3)}(\vec{r}_{ij}, \vec{r}_{ik}, \vec{r}_{jk}) \quad (3)$$

$\vec{r}_1, \vec{r}_2 \ldots \vec{r}_N$ are coordinates of the atoms. $V_{(2)int}$ is the twin potential (4); $V_{(3)int}$ tree-part *SW*-potential :

$$V_{\text{int}}^{(2)}(\vec{r}_{ij}) = \left\{ A\left(B\frac{1}{r_{ij}^p} - 1\right) \exp\left(\frac{\Lambda}{r_{ij} - a}\right) \right\}, \vec{r}_{ij} < 2{,}5\sigma_{AB} \\ 0, others \quad (4)$$

$$V_{\text{int}}^{(3)}(\vec{r}_{ij}, \vec{r}_{ik}, \vec{r}_{jk}) = \Pi_{ijk} + \Pi_{kij} + \Pi_{jki}$$

$$\Pi_{ijk} = \Lambda\left(\cos\theta_{jik} + \frac{1}{3}\right)^2 \exp\left(\frac{\delta_{ijk}}{r_{ij} - a} + \frac{\delta_{ijk}}{r_{ik} - a}\right) \quad (5)$$

Θ_{ijk} is angle, $\vec{r}_{ij}$ and $\vec{r}_{jk}$, $\vec{r}_{ij} = \left|\vec{r}_i - \vec{r}_j\right|$ is the vector between i and j atoms in units of the equilibrium distance between nearest atoms in the structure ($\vec{r}_0$). For *Si* $\vec{r}_0$ *= 2,351A (*modified SW*),* and $\vec{r}_0$*=2,0951A* (original SW). The energy unit equal *E = 2,1675* eV *i.e* $E_{Si\text{-}Si}$ in the crystal *Si* . The parameters of the modified SW-potential are present in the [3].

→Graphic Package is a geometrical program based on *3D*-representation of the investigation of NC.

We will report the results of test calculation for adsorption processes**,** optics properties of the closely packed and ball-like Si NC. Real surface objects may be built by introducing stereochemistry, i.e., the 3D atomic positions, and it is important to visualize them as molecular models with the usual rendering techniques leading to 3D perception. MMGP visualization allows investigators to emphasize at length the different aspects of molecular structure of surface: chemical topology, conformational details, etc.

We applied the MMGP to the Si-SDP. With the appearance of semiempirical methods the calculation of the equilibrium geometry and visualization of quite large model became possible (*N=125* Atoms). The calculation bond lengths of some surface are given in ref. [5-7].

As one can see from these data the calculated interatomic are in a quite good agreement with the experimental ones. Especially, the changes of the Si - Si bond, going from a small Si -NC (2-10 atoms) to big are accurately described. We find the energies of NC, binding energy per atom and interection energy of the systems «NC-SDP» are

obtained for more stable geometry. Furthermore, the energetic positions and equilibrium distances as well as of silicon are described rather well.

Other example of the adsorption process and chemical reactions on semiconductor surfaces is the interaction with halogen-atoms [6]. When using the model to represent the SDP, a choice has to be made about the NC size, that is, the number of atoms which are treated explicity in the calculation, and the level of precision of the required computation. Fortunately, the chemisorption of atoms on SDP seems to be of local character. This fact is greately supported by ab initio model calculations, and particularly by the calculations for the chemisorption of F and Cl on Si-SDP.

In our calculation the single NC contains 10-100 Si atoms, representing the first four layers of the Si-SDP. We regard this model as hypothetical molecules (quasimolecules) and do try to compare the computed results (for example, magic numbers) directly to experimental data of the corresponding impurities in the solids or chemisorbed systems [1]. The mass spectra of charged NC, where magic numbers are observed [3].

Take into account the internal structure of the ball-like Si NC we investigate theoretically the adsorbtion and scattering of light by ones. The theory for the interaction of electromagnetic fields with local charge-carrier near boundary of the small spherical semiconductor microcrystals was presented in [8]. In the [5,8] the dipole moments of NC (using MMGP) and transition dipole moments for local bulk states and local exterior surface states were calculated. It was shown that the dipole moments of the transitions for local states of the Si NC are large compared to the typical values of transition dipole moments for Si - NC.

Conclusion. We have shown that the calculated energy and geometrical characteristics by MMGP are in satisfactory agreement with the experiment and others ab initio calculations [1-8]. The present calculations show that the MMGP can be used to obtain a detailed and reasonably accurate description of various aspects of the small halogen-Si-NC. In view of interest of a physicist for the visualization of such NC, one may foresee that the data banks that represent the major types of stable systems will soon be available. Therefore, it is important for a physicist to have at hand the computer tools allowing visualization and generation of computational information. The combination MMGP with molecular dynamics in connection with technique of simulated annealing, makes it a very useful tool for the determination of geometries of large NC. Reconstruction processes at Si SDP or amorphous solids can be studied also in this way

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Abstract

The theoretical approach of quantum-dimensional system we have discussed. Our results are important for visualization and generation nanodimensional parts of the optical system.

Key words: visualization, optic, system

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НАНОЕЛЕКТРОННІ МАТЕРІАЛИ ДЛЯ ОПТИЧНИХ СИСТЕМ

Резюме

Наведені теоретичні підходи вивчення квантово-розмірних систем. Результати є важливим для візуалізації та створення нанорозмірних складових оптичних систем.

Ключові слова: візуалізація, оптика, система

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НАНОЕЛЕКТРОННЫЕ МАТЕРИАЛЫ ДЛЯ ОПТИЧЕСКИХ СИСТЕМ

Резюме

Приведены теоретические подходы изучения квантово-размерных систем. Результаты могут быть использованы для визуализации и создания наноразмерных составляющих оптических систем.

Ключевые слова: визуализация, оптика, система