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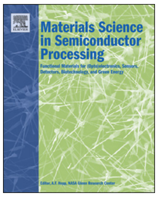

Semi-empirical tight binding method for calculating energy levels of hydrogenated silicon nanoclusters as a function of size

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ABSTRACT

A semi-empirical tight binding model is used for calculating energy levels of spherical hydrogenated silicon nanoclusters in the form of Si_mH_n and two independent bases. The first basis is the nearest neighbor approximation of sp^3s^* orthogonal basis and the second basis is the third nearest neighbor approximation of sp^3 nonorthogonal basis. Also, bulk properties of silicon crystal are used in the calculations. As we expected, obtained results show that the change in the size of nanoclusters has a great influence on their energy levels. So optical properties of these nanoclusters can be controlled externally. A comparative study on the calculated results and experimental results also reveals a good agreement between the two approaches.

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1. Introduction

Quantum nanoclusters are made of atoms with interatomic forces, and they are very useful formation of atoms. Recently, scientists have been very interested in the investigation of quantum nanoclusters and their properties [1–3]. Development of electrical industries has made scientists investigate small-sized structures to produce devices with better quality and efficiency, and semiconducting nanoclusters are one of the best choices for this reason. So semiconducting nanoclusters are very good candidates for fabricating optical [4] and electrical [5] devices.

Size is a key factor in nanoclusters. In small-sized nanoclusters, changing even one atom has important effects on nanoclusters and their properties. Unlike the molecular state, nanoclusters can be grown to larger sizes. Also, there are high surface effects in nanoclusters [6]. The ratio of surface atoms to volume atoms is considerable, so the surface effects cannot be omitted. But, in large nanoclusters, this ratio becomes smaller and the behavior of a nanocluster is similar to its bulk state's behavior. In nanoclusters where their surfaces are saturated with atoms like hydrogen, oxygen and so on, they do not have free links on their surfaces, so they are considered as tiny pieces of a bulk structure. Therefore, some bulk properties can be applied to this kind of nanoclusters.

Moreover, nanoclusters can be made in different states of matter, including solid, liquid, gas, and plasma [7]. According to the non-periodic potential of nanoclusters, they have energy levels instead of energy bands [8,9]. Knowing the energy levels of nanoclusters, investigation of their optical properties like absorption, emission, refraction, luminescence and scattering become important [10]. Because of dependence of the energy levels of nanoclusters on their sizes, these optical properties of theirs depend on their sizes too [11]. Therefore, the energy gap between the highest occupied orbital and the lowest unoccupied orbital is a variable parameter, and it can be controlled externally by adding or subtracting atoms. Thus

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the emitted or absorbed wave length of light of nanoclusters can be controlled externally.

Investigation of optical properties of a nanocluster requires obtaining of the energy levels of that nanocluster accurately. Our purpose in this work is to use the semi-empirical tight binding method to calculate the energy levels and the HUMO–LUMO energy gap of hydrogenated silicon nanoclusters in the wide range of sizes. Silicon as the most important semiconducting matter is widely used in electrical and optical industries. Silicon nanoclusters are very active optical materials, because they have direct energy gap instead of indirect energy gap of silicon bulk. So the absorption and emission of light in silicon nanoclusters are easier than in silicon bulk.

There are some other similar works on this subject [12]. These works are limited to small-sized nanoclusetrs. Due to more tight binding parameters, calculating the energy levels for bigger nanoclusters using these works was very time consuming and needed powerful computer clusters, but in this work, we have used two different bases that reduce the number of tight binding parameters for calculating the energy levels. So this method can be performed easily for medium-sized and even larg-sized nanoclusters faster and cheaper than other similar theoretical works. The only remaining issue in this work was the accuarcy of calculations. Therfore, we compared our results with some experimental results and saw that there was a very good agreement between these two results. So this method is a highly fast and reliable method for calculating energy levels of semiconducting nanomaterials like silicon nanoclusters in a wide range of sizes.

2. Semi empirical tight binding method for calculating energy bands of Si

A published paper by Slater and Koster [13] caused to use the tight binding method has been considered as a very powerful method for finding the electronic structure of crystals. Although this method possesses lower accuracy in comparison to ab initio methods, it has higher speed in the calculation of energy band structure. In this method, the Hamiltonian and overlap matrix elements are enough for solving the problem. Also, localized atomic wave functions are used for making corrections to the model of isolated atoms. The potential of lattice is very strong, so every electron is located on a single atom. The wave function of atoms have small overlap, so only the effects of near neighbors of each atom are considered. In this paper, we have used the independent electron approximation and have eliminated the exchange term.

The Hamiltonian of a crystal in the vicinity of any atom is approximated by the atomic Hamiltonian H_{at}

$$H_{at}\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r}). \tag{1}$$

$\psi_n(\mathbf{r})$ is the atomic wave function of the crystal in the vicinity of any atom, and with variation of $\mathbf{r}$, $\psi_n(\mathbf{r})$ will be variated. The whole Hamiltonian of the crystal is

$$H = H_{at} + \Delta U(\mathbf{r}). \tag{2}$$

$\Delta U(\mathbf{r})$ provides all corrections to the periodic potential of the crystal. The wave function of the whole crystal which satisfies Bloch's theorem is [14]

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{n\mathbf{R}} b_n e^{i\mathbf{k}.\mathbf{R}}\psi_n(\mathbf{r}-\mathbf{R}). \tag{3}$$

where $\mathbf{R}$ is the position of each atom in the lattice. $\mathbf{k}$ has N amount in the first Brillouin zone, consistent with the Born-von Karman periodic boundary condition. According to Eq. (3), in this method, the summation on variable n is the linear combination of atomic orbitals (LCAOs). Using Hamiltonian Eq. (1) and substituting wave function (3) instead of $\psi_n(\mathbf{r})$ and the Hamiltonian Eq. (2) instead of H_{at} and then multiplying both sides by $\psi_m^*(\mathbf{r}-\mathbf{R}')$, and

Table 1
Hamiltonian matrix of silicon crystal in the sp^3s^* basis with the nearest neighbor approximation.

	$\lvert\mathbf{s},\mathbf{R}\rangle$	$\lvert\mathbf{p_x},\mathbf{R}\rangle$	$\lvert\mathbf{p_y},\mathbf{R}\rangle$	$\lvert\mathbf{p_z},\mathbf{R}\rangle$	$\lvert\mathbf{s^*},\mathbf{R}\rangle$	$\lvert\mathbf{s},\mathbf{R}'\rangle$	$\lvert p_x,\mathbf{R}'\rangle$	$\lvert p_y,\mathbf{R}'\rangle$	$\lvert p_z,\mathbf{R}'\rangle$	$\lvert s^*,\mathbf{R}'\rangle$
$\lvert\mathbf{s},\mathbf{R}\rangle$	$E(s)$	0	0	0	0	$V(s,s)g_0$	$V(s,p_x)g_1$	$V(s,p_y)g_2$	$V(s,p_z)g_3$	0
$\lvert\mathbf{p_x},\mathbf{R}\rangle$	0	$E(p_x)$	0	0	0	$-V(p_x,s)g_1$	$V(x,x)g_0$	$V(x,y)g_3$	$V(x,y)g_2$	$-V(p_x,s^*)g_1$
$\lvert\mathbf{p_y},\mathbf{R}\rangle$	0	0	$E(p_y)$	0	0	$-V(p_y,s)g_2$	$V(x,y)g_3$	$V(y,y)g_0$	$V(x,y)g_1$	$-V(p_y,s^*)g_2$
$\lvert\mathbf{p_z},\mathbf{R}\rangle$	0	0	0	$E(p_z)$	0	$-V(p_z,s)g_3$	$V(x,y)g_2$	$V(x,y)g_1$	$V(z,z)g_0$	$-V(p_z,s^*)g_3$
$\lvert\mathbf{s^*},\mathbf{R}\rangle$	0	0	0	0	$E(s^*)$	0	$V(s^*,p_x)g_1$	$V(s^*,p_y)g_2$	$V(s^*,p_z)g_3$	0
$\lvert\mathbf{s},\mathbf{R}'\rangle$	$V(s,s)g_0^*$	$-V(p_x,s)g_1^*$	$-V(p_y,s)g_2^*$	$-V(p_z,s)g_3^*$	0	$E(s)$	0	0	0	0
$\lvert\mathbf{p_x},\mathbf{R}'\rangle$	$V(s,p_x)g_1^*$	$V(x,x)g_0^*$	$V(x,y)g_3^*$	$V(x,y)g_2^*$	$V(s^*,p_x)g_1^*$	0	$E(p_x)$	0	0	0
$\lvert\mathbf{p_y},\mathbf{R}'\rangle$	$V(s,p_y)g_2^*$	$V(x,y)g_3^*$	$V(y,y)g_0^*$	$V(x,y)g_1^*$	$V(s^*,p_y)g_2^*$	0	0	$E(p_y)$	0	0
$\lvert\mathbf{p_z},\mathbf{R}'\rangle$	$V(s,p_z)g_3^*$	$V(x,y)g_2^*$	$V(x,y)g_1^*$	$V(z,z)g_0^*$	$V(s^*,p_z)g_3^*$	0	0	0	$E(p_z)$	0
$\lvert\mathbf{s^*},\mathbf{R}'\rangle$	0	$-V(s^*,p_x)g_1^*$	$-V(s^*,p_y)g_2^*$	$-V(s^*,p_z)g_3^*$	0	0	0	0	0	$E(s^*)$

$g_0(\mathbf{k}) = \cos(k_xa_l/4)\cos(k_ya_l/4)\cos(k_za_l/4) - i\sin(k_xa_l/4)\sin(k_ya_l/4)\sin(k_za_l/4).$

$g_1(\mathbf{k}) = -\cos(k_xa_l/4)\sin(k_ya_l/4)\sin(k_za_l/4) + i\sin(k_xa_l/4)\cos(k_ya_l/4)\cos(k_za_l/4).$

$g_2(\mathbf{k}) = -\sin(k_xa_l/4)\cos(k_ya_l/4)\sin(k_za_l/4) + i\cos(k_xa_l/4)\sin(k_ya_l/4)\cos(k_za_l/4).$

$g_3(\mathbf{k}) = -\sin(k_xa_l/4)\sin(k_ya_l/4)\cos(k_za_l/4) + i\cos(k_xa_l/4)\cos(k_ya_l/4)\sin(k_za_l/4).$

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