Physics

Novel Approach to Estimation of Ground State Energies of Shallow and Deep Donors in Tetrahedrally Bonded Semiconductors

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ABSTRACT. A unified model of the impurity center is suggested. Thereupon ground state energies of the substituent donor impurities in tetrahedrally coordinated semiconductors (Ge, Si, SiC, and some $A^{III}B^{V}$ type binary compounds) are calculated on the assumption that *sp^3* hybridized bonding is realized. A simple formula, taking into account the chemical nature of the impurity useful in both cases of shallow and deep levels, is obtained. Theoretical estimates are found to be in satisfactory agreement with available experimental data. Internal contradiction, peculiar to the hydrogen-like model, is discussed. *© 2008 Bull. Georg. Natl. Acad. Sci.*

Key words: *semiconductor, impurity.*

1. Introduction

As is known, the V group atoms (like P, As, Sb, Bi) substituting for Ge or Si in IV group elemental semiconductors lead to shallow donor levels inside the band gap. Their values, found by thermal and optical measurements (for instance, see [1]), are given in Table 1. The physical mechanism of creation of such levels is as follows. Four valence electrons of the impurity atom saturate bonds with nearest neighbor lattice atoms while the fifth have to be in weekly bonded state with low ionization potential corresponding to the impurity energy level.

Essentially the same mechanism works when Ge or Si atoms are substituted by the VI group elements (like S, Se or Te) with the only difference that they form two levels in the band gap as they have two unsaturated valence electrons. The deeper level corresponds to

Table 1.

Experimental ionization potentials of the shallow donor impurities in Ge and Si

Semiconductor	Impurity	Thermal value, eV	Optical value, eV
Ge	P	0.0120	0.0125
	As	0.0127	0.0140
	Sb	0.0096	0.0102
	Bi	0.0125	0.0127
Si	P	0.0440	0.0453
	As	0.0490	0.0535
	Sb	0.0390	0.0425
	Bi	0.0690	0.0710

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1972	1974	1975	1976	1977	1978	1979	1980
0.25		0.23		0.249	0.2		0.2
	0.26		0.26		0.3	0.26	0.29
0.40							
				0.525		0.50	0.52
	0.62						

Fig. 1. Survey of published data for the energy positions from the conduction band edge of Se related centers in Si (in eV) [9].

1959	1962	1966	1970	1971	1971	1972	1976	1978	1980
		0.11	0.11						
0.18	0.19	0.19	0.19						0.2
					0.30	0.26		0.30	0.30
0.37	0.37	0.37	0.36	0.37			0.36		
					0.57	0.57	0.56		
		0.61				0.65	0.64		

Fig. 2. Survey of published data for the energy positions from the conduction band edge of S related centers in Si (in eV) [12].

single-ionized impurity atom (i.e. S^+, Se^+ or Te^+). The energy levels of the VI group impurities in Si had been determined in [2 14]. In particular, in [9,12] the dark-conductivity, photoconductivity, photo- and thermally stimulated currents, absorption, transient and thermally stimulated capacitance, MOS-technique, TSC and DLTS data for Si<S> and Si<Se> were displayed in the form of time trends. They are shown in Figs. 1 and 2.

As for the Si<Te>, there are fixed [13,14] four levels at 0.190, 0.364, 0.385 and 0.410 eV. The levels at 0.190 and 0.410 eV are identified as the ground state energies of Te and Te^+ impurity centers while the values of 0.364 and 0.385 eV should correspond to the transitions of the Te^+ center from $1SA_1$-configuration to the $2P_0$- and $2P_{\pm}$-configurations. The experimental values of the S, Se and Te deep levels in Ge are given in [15 22]. These results (according to [19]) are shown in Fig. 3.

The experimental ground state energies of donor impurities in tetrahedrally bonded $A^{III}B^V$ and $A^{IV}B^{IV}$ compounds are given in [1,22 25]. From Table 2 one can see that in one case more than 2 levels (namely 3) are obtained. Evidently, part of the obtained levels do not correspond to the substitution, but they arise from the complexes of impurity atoms with certain structural defects. The mechanism of the creation of substituting levels is same as is in Ge and Si. If IV or V (VI or VII) group impurities substitute for III (V) group atom respectively

Ge<S>	Si<S>	Ge<Se>	Si <Se>	Ge<Te>	Si<Te>
				0.093	
					0.199
0.280		0.268			
	0.318		0.307	0.332	
		0.512			0.411
0.590				0.593	
		0.618			

Fig. 3. Comparison of energy positions from the conduction band edge of the isolated chalcogen centers in Ge and Si (in eV) [19].

Table 2

Experimental ground state energies of donor impurities in tetrahedrally bonded $A^{III}B^V$ and $A^{IV}B^{IV}$ compounds (in eV)

Impurity	SiC		GaP	GaAs	GaN	InP	InSb	BN
	6H	4H						
S			0.104	0.0061		0.0057	0.0007	0.41
Se			0.102	0.0059		0.0057	0.0007	
Te			0.090	0.0058		0.0057	0.0007	
Ge				0.0060				
Si			0.088	0.0058	0.022			0.24
Sn			0.065					
N	0.081 0.138 0.142	0.052 0.092						
O		0.30 0.44			0.034			
P	0.085 0.135							

one or two electrons remain in donor state. Here we consider only the impurities with s- and p-valence electrons bonded with neighbors by the sp^3-hybridization.

Theoretical determination of the donor impurity energy spectra in semiconductors has a history of at least 70 years and quite a few studies have been devoted to this problem. The hydrogen-like atom model was the first that had been suggested for the shallow impurities. The Hamiltonian of this model consists of two terms – the crystalline Hamiltonian $H^{(0)} = -(\hbar^2/2m)\Delta - e\varphi(\vec{r})$ with periodic potential $\varphi(\vec{r})$ in the form of a superposition of constituent atoms potentials centered at the regular lattice sites and the difference $-e(\varphi_j^{(0)}(r) - \varphi_j(r))$, where $\varphi_j^{(0)}$ and $\varphi_j(r)$ respectively are the atomic potentials of the regular and substituting atoms at the j-site. Within the effective mass approximation $H^{(0)}$ is presented as $-(\hbar^2/2m^*)\Delta$. Here m^* stands for the electron effective mass. The criterion of validity for such approximation is potential smoothness – its low variation at the distances comparable with the lattice constant. Initially the ground state energy of the donor impurity was calculated by Mott and Henry [26], presenting the above mentioned potential difference by the hydrogen-like potential $-e^2/\varepsilon r$, where ε denotes the static dielectric constant of the bulk semiconductor. Thus, the problem is simplified and reduced to the determination of the energy spectra of quasi-particle with effective mass of m^* and effective charge of $e/\sqrt{\varepsilon}$ affected by the Coulomb potential. It immediately gives $E = (m^*/m)E_H/\varepsilon^2$, where $E_H = -13.6$ eV is the ground state energy of the hydrogen atom. The radius of the donor electron orbit equals $a = (m/m^*)\varepsilon a_0$, where $a_0 = 0.53$ Å is the Bohr radius. The application of the hydrogen-like model within the effective mass approximation is allowed if the radius a is many times greater than the lattice constant d. A model of this kind is well acceptable for Ge<As> or Si<P>. Further the issue has been discussed, using more refined approximations. Kohn and Luttinger [27] and Kitten and Mitchell [28] considered effective mass dependence upon the direction introducing the effective mass tensor. Ansel'm and Korovin [29] took into account the tensor nature of the dielectric permittivity as well. The problem of the shallow impurities energy spectra in frames of hydrogen-like model within the effective mass approximation was considered by Foulkner [30], using the variation method. The results obtained for excited levels in Ge and Si are the best among available theoretical ones. But, it is not true for the ground state energy values [31].

As was seen, the singly-ionized VI group atoms form deep levels in the gaps of Ge and Si. Nevertheless, the physical mechanism of formation is quite the same as in the case of the shallow levels arisen from the V group impurities. The only difference is related to the central charge Z. For shallow levels $Z = 1$, while for deep ones $Z = 3$. The validity of the hydrogen-like model approach is satisfied in both cases. Moreover, for the deep levels in Ge the criterion is met better ($a \approx 49a_0$ and $d \approx 11a_0$) than for shallow levels in Si ($a \approx 45a_0$ and $d \approx 10a_0$). But, in both cases the calculated deep levels are markedly distinguished from the measured ones. Thus, there exists an intrinsic contradiction in the hydrogen-like model and in the suggested form it can not be applied. The good results obtained for shallow levels, using hydrogen-like model, may be considered as accidental. Below we will try to explain why such a situation takes place.

Owing to this the quantitative description of the photo-transitions via the various impurity centers can be attained only in different models. For instance, the impurity potential suitable for deep levels is presented by the Lukovsky model [32], while for the intermediately lying levels within the quantum defect model [33] etc. So, different theoretical approaches are necessary, despite the fact that these defects differ one from another only by the charge numbers.

2. Calculation of the donor impurities ground state energy

Beginning with the 1970s a series of investigations appeared in which the impurity center Coulomb-like potential is corrected, taking into account the dielectric constant spatial distribution $\varepsilon(r)$. This dependence on Ge and Si was studied by a number of authors [34 37]. It was shown that when $r \to 0$ the dielectric constant value $\varepsilon(r) \to 1$ while at $r > r_0$, i.e. outside the first coordination sphere with radius of r_0, $\varepsilon(r) \approx \varepsilon$. This encouraged us to separate the first coordination sphere from the remainder space and approximate $\varepsilon(r)$ as [38]

$$\varepsilon(r) = \theta(r_0 - r) + \theta(r - r_0)\,\varepsilon \tag{1}$$

Here θ denotes the Heaviside step-function. Consequently, inside the first coordination sphere the bound electron is considered as moving in vacuum. Accordingly, its mass is equated with the free electron mass. The effective mass is introduced only for characterization of the electron transfer between different atoms. Besides, inside the first coordination sphere it is as-

sumed that the electron interacts only with the central impurity ion and four neutral neighbor regular atoms. The interactions with the remaining atoms of the lattice are neglected as they are neutral and at $r \le r_0$ their potentials are too weak in comparison with the mentioned potentials. As for the space outside the first coordination sphere, the electron motion is described in a common way, within the continuum approximation.

As is known [39], in tetrahedrally coordinated crystals the interatomic bonding is realized through the sp^3 hybridized orbitals $\Phi_i(r)$,

$$\Phi_1(r) = \frac{1}{2}\Psi_s(r) + \frac{\sqrt{3}}{2}\Psi_{px}(r),$$

$$\Phi_2(r) = \frac{1}{2}\Psi_s(r) - \frac{1}{2\sqrt{3}}\Psi_{px}(r) + \sqrt{\frac{2}{3}}\Psi_{pz}(r),$$

$$\Phi_3(r) = \frac{1}{2}\Psi_s(r) - \frac{1}{2\sqrt{3}}\Psi_{px}(r) + \frac{1}{\sqrt{2}}\Psi_{py}(r) - \frac{1}{\sqrt{6}}\Psi_{pz}(r),$$

$$\Phi_4(r) = \frac{1}{2}\Psi_s(r) - \frac{1}{2\sqrt{3}}\Psi_{px}(r) - \frac{1}{\sqrt{2}}\Psi_{py}(r) - \frac{1}{\sqrt{6}}\Psi_{pz}(r). \quad (2)$$

In the case under consideration, $\Psi_s(r)$ is the s-orbital of the impurity atom valence shell while $\Psi_{px}(r)$, $\Psi_{py}(r)$, and $\Psi_{pz}(r)$ are the components of the p-orbital of the same shell. Within the LCAO-approximation the donor electron wave function inside the first coordination sphere can be constructed using sp^3-hybridized wave functions as a basis set:

$$\Psi_1(r) = \sum_{i=1}^{i=4} C_i \Phi_i(r) \qquad r \le r_0. \quad (3)$$

Here $|C_i|^2$ represents the probability of the i-electron detection. Four electrons (from the five) of the single- (or twice-) ionized V (or VI) group atom are involved in bonding, while the fifth (donor) electron can be captured on one of the orbits with equal probability, $|C_1|^2 = |C_2|^2 = |C_3|^3 = |C_4|^2$. According to the normalizing condition $|C_1|^2 + |C_2|^2 + |C_3|^3 + |C_4|^2 = 1$ and taking into account the bonding maximality condition [39], we get $C_1 = C_2 = C_3 = C_4 = 1/2$. Consequently,

$$\Psi_1(r) = \Psi_s(r) \qquad r \le r_0. \quad (4)$$

Therefore the donor electron inside the first coordination sphere is in s-state. In our opinion, this is the reason why the ground state energy values in Ge and Si reveal growing and decreasing trends which in chemistry are called "secondary periodicity" [40]. Such periodicity is characteristic of the first ionization energies of the elements with s-electrons on the outer shell, belonging to the same group as the above mentioned ones. For instance, these are the I group elements Na, Cu, Ag, and Au; and also the II group elements Mg, Zn, Cd, and Hg. The secondary periodicity becomes sharper expressed when the number of outer shell electrons increases. The same trend is characteristic of the terms of P, As, Sb, and Bi impurities [41,42]. Below, the requirement of the periodicity maintenance will be discussed in connection with the impurity levels identification problem.

Let us take the electron wave function inside the first coordination sphere ($r \le r_0$) in the form of the outer shell s-state orbital expressed by the Slater-type wave function [43]

$$\Psi_1(r) \equiv \Psi_s(r) = A r^{n^*-1} \exp(-Z^* r / n^* a) \quad r \le r_0, \quad (5)$$

where A is the normalizing factor, while n^* and Z^* are the effective quantum number and effective charge number, respectively. These parameters, estimated from the Slater-rules, show up to 30-40 % deviations from their experimental values [43]. This is the reason why below we will suggest a different way of determination. The theoretical value of the term under consideration (i.e. s-term) we take as it was calculated [41] for the Thomas–Fermi–Dirac atom because it is in best agreement with the experimental data.

The electronic state $\Psi_2(r)$ outside the first coordination sphere ($r \ge r_0$) may be described on the basis of Schrödinger's equation within the effective mass approximation

$$\left(-\frac{\hbar^2}{2m^*} - \frac{Ze}{\varepsilon r}\right)\Psi_2(r) = E\Psi_2(r) \qquad r \ge r_0. \quad (6)$$

Its solution is as follows [43]

$$\Psi_2(r) = B(na_0 / 2r) W_{n,1/2}(2r / na) \quad (7)$$

where $W_{n,1/2}$ is the Whittaker function, n is the principal quantum number, and B is the normalizing factor. For the ground state (i.e. for n = 1) it is reduced to the expression

$$\Psi_2(r) = B\exp(-\lambda r) \quad (8)$$

where $\lambda = (m^* / m)\varepsilon a_0 / Z$.

Sewing together at the boundary $r = r_0$ the wave

functions (5) and (8) and applying the normalizing condition, we find the values of the A and B factors and then according to the formula $E = \int d\vec{r}\Psi^*(r)H(r)\Psi(r)$ calculate the ground state energy. After intricate but simple transformations we get

$$\frac{E}{E_H} = 1 + \frac{2Z}{\varepsilon}\frac{Z^{*2}}{n^{*2}}\frac{m^{*2}}{m^2}\frac{r_0^3}{a_0^3}\left(1 - \frac{2Z}{\varepsilon}\frac{m^*}{m}\frac{r_0}{a_0}\right). \quad (9)$$

According to the Slater-method the n^*-state electron energy in free atom with effective charge of Z^* equals $I \equiv E_{n^*Z^*} = (Z^*/n^*)^2 E_H$. Consequently, using the given term value I one can find the $Z^*/n^* = \sqrt{I/E_H}$ ratio and therefore avoid the error that arises when this quantity is determined directly by the Slater-rules. Finally, the donor electron ground state energy is found in the form of

$$\frac{E}{E_H} = \frac{Z^2}{\varepsilon^2}\frac{m^*}{m}\left(1 + \frac{2I}{E_H}\frac{m^{*2}}{m^2}\frac{r_0^3}{a_0^3}\left(1 - \frac{2Z}{\varepsilon}\frac{m^*}{m}\frac{r_0}{a_0}\right)\right). \quad (10)$$

The obtained expression includes the chemical individuality of the impurity atom via the outer shell s-term I. Its value is taken from [41] where the corresponding dependence of the s-state term on the atomic number was shown. These curves were plotted using various theoretical approaches, like Thomas–Fermi, Thomas–Fermi–Dirac, Hartree, and Hartree–Fock methods. Also the experimental values were shown. One can find that there is a good agreement between theoretical results obtained by the Thomas–Fermi–Dirac calculations and experimental data. This is the reason why we consider it more reliable than later ones [42, 44]. For instance, according to [42] the ratio error for K 2*s*-, Sr 4*s*-, and Ba 5*s*-terms consists of 47, 37, and 90 %, respectively.

As for the electron effective mass, in semiconductors with the anisotropic quadratic dispersion-law the averaged electron effective mass is determined ambiguously [40,45,46]. According to Tsidilkovskij [47], in the problem under consideration the averaged mass is the density-of-state mass, while according to [48] this is the mass of conductivity. Besides, the electron migration averaged effective mass determination [40] leads to

$$\frac{m}{m^*} = 1 + \frac{2m\gamma^2 V_2^2 r_0^2}{3\hbar^2 E_0} \quad (11)$$

with $E_0 \approx 3.60\,(\sqrt{V_2^2 + V_3^2} - 1.11V_1)$. Here V_1, V_2, and V_3 are the metallic, covalent, and ion binding energies, respectively; γ is the scaling factor which takes on values of 1.60 (Ge), 1.40 (Si), 1.26 (SiC), 1.50 (GaP), 1.13 (BN) etc. Using them according to the stated formula (11) we find the electron migration effective mass values m^*/m in various semiconductors: 0.173 (Ge), 0.264 (Si), 0.437 (SiC), 0.310 (GaP), 0.510 (BN). All parameters needed for calculation are summarized in Table 3. On the basis of these parameters, using the obtained formula, we have calculated the donor impurities ground state energy. They are listed in Table 4.

3. Results analysis and identification of some impurity levels

Let us begin from the analysis of Ge and Si. As one can see, for both materials the values calculated by the obtained formula (taking into account the impurities individuality through the “chemical shifts”) are in good agreement with corresponding experimental data.

As for the deep impurities Si<S$^+$> and Si<Se$^+$>, the same formula (10) provides good agreement for most part of the experimental results shown in Figs. 1 and 2. We disagree with the results suggested in [9,12] for Si<S$^+$> and Si<Se$^+$>. According to these works, the mentioned impurity levels are 0.618 and 0.593 eV. But, defect identification seems to be wrong as energy values do not follow the secondary periodicity trend, which is obligatory as S$^+$, Se$^+$, and Te$^+$ defects differ from P, As, and Sb only by the central charge value. In general, the s-electrons of the atomic valence shell are characterized by secondary periodicity like P, As, and Sb (which retain this trend to be inserted into lattice). On the other hand, Figs. 1 and 2, respectively, show that according to most experimental data the Si<S$^+$> level lies at 0.36 – 0.37 eV and the Si<Se$^+$> level lies at 0.50 – 0.52 eV. From the values 0.190, 0.364, 0.385, and 0.410 eV, suggested in [13], for Si<Te$^+$> the level 0.364 eV is in better agreement with our result. Thus our results 0.356, 0.450, and 0.343 eV

Table 3

Electron migration effective mass, dielectric constant and radius of the first coordination sphere in tetrahedrally-bonded semiconductors

	Ge	Si	SiC	GaP	GaAs	GaN	InP	InSb	BN
m^*/m	0.173	0.264	0.438	0.310	0.067	0.13	0.07	0.014	0.510
ε	16.0	12.0	10.0	10.1	12.5	9.7	12.5	16.0	7.1
r_0/a_0	4.6	4.4	3.6	4.4	4.6	3.7	4.8	5.3	3.0

Table 4

Calculated ground state energies of the donor impurities in tetrahedrally bonded semiconductors (in eV)

Impurity	Atom	Ge	Si	SiC	GaP	GaAs	GaN	InP	InSb	BN
P	15.7	0.0127	0.047	0.145						
As	23.8	0.0145	0.058							
Sb	14.0	0.0123	0.044							
Bi	22.0	0.0141	0.056							
S	19.5				0.104	0.0067		0.0069	0.00074	0.38
S^+	30.0	0.0820	0.356							
Se	29.1				0.134	0.0070		0.0072	0.00075	
Se^+	42.0	0.1010	0.450							
Te	18.0				0.099	0.0063		0.0068	0.00074	
Te^+	27.0	0.0780	0.343							
Ge	21.1				0.120	0.0068		0.0069	0.00074	
Si	13.0				0.083	0.0062	0.0217	0.0066	0.00074	0.29
Sn	12.7				0.082	0.0062		0.0066	0.00074	
N	20.3			0.170						
O	30.3						0.0260			
O^+	44.0			0.224						
C	13.0									0.33

found for Si<S^+>, Si<Se^+>, and Si<Te^+> levels, respectively, can also be considered as satisfactory.

In the case of Ge we meet with some misunderstandings. The first is also connected with secondary periodicity: most of the earlier suggested values do not follo econd is that according to [13,14], these levels in Ge are commensurate with that in Si. For instance, there are suggested 0.590 and 0.618 eV for Ge<Te^+> and Si<Te^+>, respectively. But, as mentioned for the physically identical shallow levels, the corresponding energies in Ge are at least 4 times smaller than in Si. By reason of this, we believe that the results of [14] do not attribute to the ground state energies of the substituting impurities in Ge. The values obtained in the present work seem to be preferable.

The energy levels created inside the band gap of the SiC polytypes by the donor impurities (P, N, and O), given in Table 2, are taken from [20 25]. In all modifications the averaged electron effective mass of migration (not the effective mass of conductivity), dielectric constant, and bond lengths between nearest neighbors are nearly the same and thus our calculations lead to the same donor levels. In [25] as well as in other works we did not find complete identification of the levels listed in Table 2. Here we try partial identification. It should be mentioned that the values of 0.145, 0.170, and 0.224 eV found for SiC<P>, SiC<N>, and SiC<O>, respectively, are placed near the experimental ones of 0.135, 0.142 eV, and 0.300 eV. So, proceeding from our calculations, we conclude that these levels are attributed to P, N, and O donor impurities.

Tables 3 and 4 reveal satisfactory agreement between the calculated results and corresponding experimental data in the cases of GaP, GaAs, GaN, InP, and InSb.

Now let us return to the issue why the hydrogen-like model with internal contradiction yields more or less satisfactory results in the case of shallow levels. From the obtained formula it follows that at $Z = 1$ the second term is small in comparison with 1 and thus leads to the small correction like “chemical shift”. Consequently, in the case of shallow impurities electron does not “feel” (or weakly “feels”) a strong field inside the first coordi-

nation sphere, which in behavior differs from the Coulomb-like field. But, when $Z = 2$, i.e. in the case of deep level, the mentioned term exceeds 1 and short-ranged potential of the impurity center is a determinant for electron moving.

4. Conclusions

The present work has claims neither to precise calculations nor to the general solution of the shallow and deep impurities energy spectrum problem. We suggest a unified description of the energy states of shallow and deep substituting impurities in semiconductor materials with tetrahedral sp^3-hybridized bonds. For this purpose we propose an impurity center model which was elaborated and realized for electron scattering by the ionized impurity centers, and radiative and nonradiative electron transitions via these defects [38,49,50]. It may be that a more precise solution will be found using recent theoretical approaches like the Wannier-function method [51,52]. However, the advantages of our approach lie in unified description found for certain shallow and deep impurity levels, taking into account the individuality of impurities and the possibility to reduce problem solution to simple analytic expressions. Besides, the obtained formula predicts the ground state energies of some impurities that have not yet been experimentally detected.

ფიზიკა

ტეტრაედრულად ბმულ ნახევარგამტარებში თხელი და ღრმა დონორების ძირითადი მდგომარეობის ენერგიების შეფასება ახლებური მიდგომით

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(წარმოდგენილია აკადემიის წევრის გ. ჩაგელიშვილის მიერ)

ნაშრომში გათვლილია გარკვეული კლასის თხელი და ღრმა მინარევების ძირითადი მდგომარეობის ენერგიები ტეტრაედრული სიმეტრიის ნახევარგამტარულ ნივთიერებებში, როგორებიცაა პერიოდული სისტემის IV ჯგუფის ნივთიერებები, A_4B_4 და A_3B_5 ტიპის ნაერთები. განხილულია ის თხელი და ღრმა მინარევები, რომლებსაც მოცემული ტიპის ნახევარგამტარული ნივთიერებების აკრძალულ ზონებში ენერგეტიკული დონის შექმნის ერთი და იგივე ფიზიკური მექანიზმი გააჩნიათ. აქვე ვრცლადაა მოყვანილი ზემოხსენებულ ზონებში თხელი და ღრმა მინარევების ენერგეტიკული დონეების ექსპერიმენტული მონაცემები. ასევე, ნაჩვენებია, რომ ამ დეფექტების ენერგეტიკული სპექტრის თეორიული გათვლების საფუძველი – წყალბადისებური ატომის მოდელი – შინაგანად წინააღმდეგობრივია.

მოცემული ამოცანის გადაწყვეტის მიზნით, ავტორების მიერ შემოთავაზებულია მინარევული ცენტრის ერთიანი მოდელი, რომლის თანახმად მინარევის ატომი პირველ კოორდინაციულ სფეროში განიხილება როგორც თავისუფალი ატომი ვაკუუმში, ხოლო მის გარეთ კი, ჩვეულებრივად, – უწყვეტი ტანის კონტინუუმის მიახლოებაში. ამავე მოდელში, LCAO მიახლოების გამოყენებით, ნაჩვენებია, რომ დონორული ელექტრონის ტალღურ ფუნქციას პირველ კოორდინაციულ სფეროში წარმოადგენს მინარევული ატომის გარე, სავალენტო შრის s-მდგომარეობის ტალღური ფუნქცია, ხოლო მის გარეთ კი — წყალბადისებური ატომის მიახლოების 1s-მდგომარეობის ტალღური ფუნქცია.

დონორული ელექტრონის ძირითადი მდგომარეობის ენერგიის პირდაპირი გათვლით მიღებული ფორმულა აღწერს როგორც თხელ, ასევე ღრმა მინარევულ დონეებს, თითოეული მინარევის ინდივიდუალობის გათვალისწინებით. მიღებული შედეგები დამაკმაყოფილებლად ეთანხმება შესაბამის ექსპერიმენტულ მონაცემებს. გარდა ამისა, მიღებული ფორმულით ახსნილია წყალბადისებური ატომის მოდელის შინაგანი წინააღმდეგობა. გათვლების შედეგად მიღებული შედეგების მიხედვით მართებულადაა იდენტიფიცირებული მინარევული დონეების ის ექსპერიმენტული მონაცემები, რომლებიც არაცალსახად, ან საერთოდ არ იყვნენ იდენტიფიცირებულნი.

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