INTERATOMIC INTERACTION IN DIATOMIC MOLECULES WITH TAKING INTO ACCOUNT THE REPULSION OF IONS IN A POSITIVELY CHARGED CORE

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Abstract:

Introduction/purpose: Different types of interactions in diatomic molecules of complex atoms are analysed.

Methods: The empirical formulas of Lennard-Jones, Buckingham, Buckingham-Corner, Morse, Danem, Gulbert-Hirschfelder, Klein and their combinations without their clear physical justification are used to take into account the repulsive and attractive forces in the molecule. To improve the situation of the binary interaction inside condensed matter, Gretchikhin and his associates proposed applying the Heitler-London quantum theory, but only at distances greater than equilibrium. At distances less than equilibrium between atoms in the binary interaction, the Lennard-Jones formula was still used. Using various kinds of fitting coefficients, in each case we obtained a match with the experimental data on the dissociation energy. A more general idea of all possible types of interactions was completely absent. In this connection, the need arose to reveal all possible types of interactions inside diatomic molecules and theoretically obtain dissociation energy, activation energy, and standard atomization enthalpy. The application of quantum mechanics methods in the Heitler-London theory allowed to take into account not only the Coulomb deterrence during exchange interaction, but also the Coulomb repulsion of nuclei.

Results: The electric dipoles for neutral atoms and for positively charged ions of the core of diatomic molecules were calculated. This made it possible to calculate the electron-dipole and dipole-dipole interactions. A theory of the repulsion of positively charged nuclei of complex atoms in diatomic molecules has been developed. The interaction potentials for the molecules of carbon, nitrogen, oxygen, aluminum, silicon, and sodium are

calculated. The developed physical model of the formation of diatomic molecules is compared with the empirical potentials of Lennard-Jones and Morse. At the internuclear distance equal to the sum of the energy radii of atoms in the molecule, a potential jump occurs with a transition from the negative to the positive region of binding energies, which determines the activation energy of the formation of diatomic molecules.

Conclusion: From the obtained interaction potentials of atoms in diatomic molecules, the activation energy, ionization energy, standard atomization enthalpy, and electron affinity are determined.

Key words: interaction potential, covalent bond, ionic bond, electric dipole, induced bond, diatomic molecule.

Introduction

The interaction of atoms is a rather complicated process. This mechanism is understood qualitatively under the assumption that there are attractive and repulsive forces between the interacting atoms. However, these forces are extremely entangled and that is why creating a model of their interaction appeared to be a difficult task. Therefore, a simpler way of applying the regression analysis to describe the interaction potential between atoms was used. As a result, Lennard-Jones, Buckingham, Buckingham-Corner, Morse, Dunham, Hulbert-Hirschfelder, and Klein potentials were obtained as well as their combinations (Hirschfelder et al, 1954). The first, quite widespread formula, representing the interaction potential, was proposed by Lennard and Jones in the following form (Gretchikhin, 2018), (Yelyashevich, 1962):

$$V(r) = -\frac{a}{r^6} + \frac{b}{r^{12}}, \tag{1}$$

where *a* and *b* constants are fitting coefficients.

The formula proposed by Dunham turned out to be more universal:

$$V(r) = V_0 \left\{ \left[b_0 \left(1 - \frac{r_0}{r} \right)^2 \right] \cdot \left[1 + \sum_{n=1}^{N} b_n \left(1 - \frac{r_0}{r} \right)^n \right] \right\}, \tag{2}$$

where: V_0 is the depth of a potential well; r_0 is the equilibrium value of the radius corresponding to the minimum interaction potential $V(r_0)$; and b_0, b_n and *n* are the fitting parameters.

For diatomic molecular systems the potential proposed by Morse is usually used (Gretchikhin, 2018):

$$V(r) = D_e \left[1 - \exp(-\beta \Delta r) \right]^2 . \tag{3}$$

The initial parameters for constructing the Morse potential are the dissociation energy D_e, the distance difference relative to the location of one of the nuclei Δr, and β, which is determined as follows: $\beta = \sqrt{o/2D_e}$. In turn, the force constant O is found from the vibrational spectrum and was obtained for most diatomic molecules.

To exclude any fitting coefficients, the paper (Gretchikhin, 2018) proposed a slightly different approach presented in the following form for the condensed systems:

$$V_{res.}(r) = \begin{cases} -\dfrac{2V_0 r_e^6}{r^6} + \dfrac{V_0 r_e^{12}}{r^{12}}, & at \quad r \le r_e; \\ \sum\limits_{i=1}^{3} N_i \kappa_i^2 \left[\sum\limits_{k=0}^{3} \sum\limits_{l=0}^{3} Z_{a,k}^* Z_{b,l}^* \int\limits_{(a)} \int\limits_{(b)} \rho_{e,a}(\varepsilon_k) \rho_{e,l}(\varepsilon_l) \left(\dfrac{H_{1,1} + H_{1,2}}{1+S} \right) d\varepsilon_k d\varepsilon_l \right] \text{at} > r_e \end{cases} \quad (4)$$

Here $V_{res.}(r)$ is the interaction potential of particles depending on the distance between the particles; $V_0 = D_e$ is the energy of interaction of the particles at the equilibrium distance which is equal to the energy of dissociation; r_e is the equilibrium distance between the interacting particles; $N_{k(l)}$ is the number of particles within the *k(l)*-th energy state; κ_i is the visibility coefficient; $Z_{a,k}^*, Z_{b,l}^*$ are effective charges of the interacting particles; $\rho_{e,a}(\varepsilon_k), \rho_{e,b}(\varepsilon_l)$ is the distribution of the electron density ρ_e of the particles around the power centers *A* and *B* of the interacting particles with the energies ε_k and ε_l in the *k*-th and *l*-th energy states; $H_{1,1}$, $H_{1,2}$ и *S* are the Coulomb, exchange, and overlap integrals, respectively.

This formation of the interaction potential between atoms in a diatomic molecule involves two problems. The first one is that the equilibrium distance is always greater than the value obtained from the analysis of the vibrational spectrum of the resulting molecule, since the repulsion energy of ions in a positively charged core is not taken into account.

The second problem arose in that the overlap integral at the equilibrium distance turned out to be greater than the unity which does not correspond to the physical nature of this integral. The integral should always be less than one.

In this connection, it is vital to set the following goal: to develop a model of the interaction of atomic structures that would allow, by applying the initial data on the ionization potentials experimentally obtained for all

atoms of the periodic table, to fully obtain the interaction potential between the atoms. To achieve this goal, it is essential to solve the following tasks:

- to find out the conditions of applicability of different types of chemical bonds that arise between the interacting atoms;
- to formulate a model of the interaction between the ions of a positively charged core;
- to develop a model of the interaction between different energy states of a positively charged core;
- to make a comparative analysis of the interaction potentials using a number of examples and taking into account the presence of covalent, ionic, induced, electron-dipole, and dipole-dipole bonds, as well as the repulsion energy of atoms and positive core ions in the initial atomic structures.

Let us consider, one after another, these problems.

A Analysis of different types of chemical bonds between interacting atoms

A fairly detailed analysis of different chemical bonds was performed in the paper (Gretchikhin, 2018). The paper shows how the following interactions are formed: covalent, ionic, induced, electron-dipole and dipole-dipole ones. However, the interactions resulting from the presence of a positive core inside the molecule were not considered.

A covalent bond is formed by the exchange of electrons between interacting particles. Heitler and London, using quantum mechanics, developed the theory of this type of interaction and applied it to the analysis of the hydrogen molecule. Figure 1 shows a schematic diagram of the electron exchange. Based on the general ideology considered in the paper (Gretchikhin et al, 1990), the exchange interaction potential in the notation shown in Figure 1 is represented in the following form:

$$U = \frac{1}{4\pi\varepsilon_0}\left(\frac{e^2}{r_e} + \frac{e^2}{r_{1,2}} - \frac{e^2}{r_{a,b}} - \frac{e^2}{r_{b,a}}\right), \tag{5}$$

where ε_0 is the dielectric constant of the vacuum while $r_{1,2}$ is the distance between the electrons.

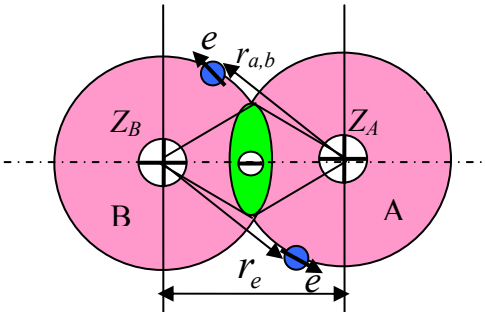

Figure 1 – Schematic diagram of the electron exchange between two identical atoms
Рис. 1 – Схема обмена электронами между двумя одинаковыми атомами
Слика 1 – Шематски приказ размене електрона између два идентична атома

In the case of the interaction of identical atoms, the exchange of electrons occurs in the zone of overlapping wave functions, which is located at a distance of $\sim r_e/2$ from both atoms. Taking into account the probability P_a of a valence electron being in the overlap zone, an electron that passes from the atom A to the atom B and is held by the electric field of the atom A has the following energy:

$$U_a^+ = P_a e^2 / 4\pi\varepsilon_0 (r_e/2).$$

A similar electron holding potential arises for the atom B:

$$U_b^+ = P_b e^2 / 4\pi\varepsilon_0 (r_e/2).$$

The resulting potential that holds the exchange of electrons for identical atoms at relatively small distances r_e is equal to $P_a \cong P_b \approx 0.5$ and therefore amounts to: $U^+ = U_a^+ + U_b^+ \cong e^2 / 4\pi\varepsilon_0 r_e$.

Based on the form of the resulting confining potential, it was thought that the potential takes into account the repulsion of the nuclei of interacting atoms. Therefore, it was believed that the Heitler-London theory already took into account the interaction of the nuclei. This mistake costs us dearly. The first term in the interaction potential (5) does not take into account the repulsion of the nuclei, but confines the electrons during the transition from one atom to another. The repulsion of

the nuclei should be taken into account separately and in a completely different way.

Potential (5) was written for a hydrogen molecule in which identical atoms interact. For diatomic molecules composed of different atoms, potential (5) has a different form and, therefore, the Heitler-London theory in this case needs to be further developed.

The direct exchange of valence electrons between the interacting particles creates the bond exchange energy in dynamics. In the process, each electron of the atom A independently interacts with all electrons of the atom B. The resulting energy of the bond was obtained in the paper (Gretchikhin, 2004)

$$E_{ков} = \sum_{k}^{N_A}\sum_{l}^{N_B}\left(\frac{H_{1,1}+H_{1,2}}{1+S}\right)_{k,l}. \tag{6}$$

Here, N_A is the number of energy levels of the particle A and N_B is the number of energy levels of the particle involved in the interaction, while the other values are as follows:

$H_{1,1} = \iint \psi_a^*(r_{a,1})\psi_b^*(r_{b,2})\widehat{H}'\psi_a(r_{a,1})\psi_b(r_{b,2})d\xi_1 d\xi_2$ is the Coulomb integral,

$H_{1,2} = \iint \psi_a^*(r_{a,2})\psi_b^*(r_{b,1})\widehat{H}'\psi_a(r_{a,2})\psi_b(r_{b,1})d\xi_1 d\xi_2$ is the exchange integral,

$S = \iint \psi_a^*(r_{a,1})\psi_b^*(r_{b,2})\psi_a(r_{a,2})\psi_b(r_{b,1})d\xi_1 d\xi_2$ is the overlap integral.

Accordingly, ψ_a and ψ_b are the wave functions of the atom A and the atom B in the ground state.

The probability of a valence electron being in the contact zone of the first and second interacting particles is determined as follows:

for the atom A $\quad P_{a,k} = 1 - \dfrac{2\alpha_k}{4\pi}$, (7)

and for the atom B $\quad P_{b,l} = 1 - \dfrac{2\beta_l}{4\pi}$. (8)

Here the angles are:

$$\alpha_k = \arctan\left(\frac{\sqrt{r_{a,k}^2 - r_{1,k}^2}}{r_{1,k}}\right) \text{ и } \beta_l = \arctan\left(\frac{\sqrt{r_{b,l}^2 - r_{2,l}^2}}{r_{2,l}}\right) \tag{9}$$

In addition, it is necessary to take into account the mutual shading of each internal energy state by external electrons. This process is taken

into account by the share in the exchange interaction of each electronic state, which should be determined as follows:

$$\delta = \frac{Z_k^* = \sum_{i=1}^{i=k-1} Z_i^*}{Z_1^*} \quad . \tag{10}$$

In the process of electron exchange, a situation arises when both electrons are near one of the interacting atoms. In this situation, an ionic bond occurs, i.e., the interaction of a negative ion with a singly ionized atom is realized.

Ionic bond. The theory of ionic bonding which makes it possible to determine quantitatively the magnitude of ionic bonding based on the residence time of valence electrons near interacting particles has been developed in the papers (Gretchikhin, 2004) and (Gretchikhin, 2008) not only for neutral particles, but also for each multiplicity of ionization.

The probability of a valence electron being in the contact zone near the first and second interacting particles is determined as follows:

for the atom A:

$$P_a = \frac{2\arctan\left(\frac{\sqrt{r_a^2 - r_1^2}}{r_1}\right)}{4\pi}, \tag{11}$$

and for the atom B

$$P_b = \frac{2\arctan\left(\frac{\sqrt{r_b^2 - r_2^2}}{r_2}\right)}{4\pi}. \tag{12}$$

Given this, the probability that the valence electron of the atom A will go over to the atom B will amount to $P_a S$ while the probability that the valence electron of the second atom is not within the contact zone amounts to (1–P_b). The resulting probability of this event is equal to $P_a S$ (1-P_b). A similar situation occurs when the valence electron of the second atom is within the contact zone and passes to the first atom while the electron of the first atom is not within the contact zone; the probability is equal to $(1-P_b)$. In this case, the probability of the event is equal to (1-P_a)·$P_b S$. Both in the first and second cases, an ionic bond arises. The

total probability of the ionic bond formation is the sum of these probabilities

$$\Theta = P_a(1-P_b)S + P_b(1-P_a)S\ . \tag{13}$$

Therefore, in the binary interaction of two identical atoms, the ionic bond energy, in general, is determined by the following formula:

$$E_{ion} = \Theta \frac{e^2}{4\pi\varepsilon_0 r_e}. \tag{14}$$

Table 1 shows, as an example, the shares of the ionic bond arising from the binary interaction of two atoms with the formation of a diatomic molecule.

Table 1 – Shares of an ionic bond and electric dipole moments for diatomic molecules
Таблица 1 – Доля ионной связи и дипольные электрические моменты для двухатомных молекул
Табела 1 – Удео јонске везе и електричних диполних момената за двоатомске молекуле

Parameter	C_2	N_2	O_2	Si_2	Al_2	Na_2
Θ (%)	16.70	10.61	33.6	13.78	43.15	30.26
$p_{э,1(2)} \cdot 10^{30}$ C·m	5.196	3.429	2.228	5.705	4.916	-
$p_{э,3(4)} \cdot 10^{30}$ C·m	3.160	2.228	3.158	2.626	-	-
$p_{э,5(6)} \cdot 10^{30}$ C·m	-	1.094	2.165	-	-	-
$p_{э,7(8)} \cdot 10^{30}$ C·m	-	-	1.184	-	-	-
EA (kJ/mol)	-	16.42	57.6	89.08	405.4	321.1

It turns out that, even for identical atoms, the fraction of the ionic bond energy is noticeable and not equal to zero.

In the process of electron exchange, an uncompensated charge arises in the region of overlapping wave functions. This charge, interacting with the positive core of the molecule, additionally increases the binding energy of the atoms in the diatomic molecule, i.e., the binding energy arises due to the induced electric charge. (Gombás, 1950)

Induced bond. An induced bond is determined by a potential barrier occurring between the interacting particles when exchanging valence electrons.

The electron of the atom A and the electron of the atom B create a negative potential barrier independently of each other. The electron when traveling from one particle to the other is partially reflected and retarded at the boundary interacting particles. The probability of such an event is equal to the product $P_a(1-P_b)(1-S)$. At the same time, the second electron is also reflected from the boundary with the probability of $P_b(1-P_a)(1-S)$. Therefore, the probability of the formation of a negative potential barrier is equal to the sum of these probabilities. Thus, the value of the negative charge in the contact zone will amount to

$$\Delta Q = [P_a(1-P_b)+(1-P_a)P_b](1-S)e. \quad (15)$$

As a result, additional binding energy arises:

$$E_{ind.} = \frac{2\Delta Qe}{4\pi\varepsilon_0 r_e}\left((1-P_a)Z_a^* + (1-P_b)Z_b^* + P_aP_a^+Z_a^{*+} + P_bP_b^+Z_b^{*+} + P_aP_a^{++}Z_a^{*++} + ...\right), \quad (16)$$

where Z_a^*, Z_b^*, Z_a^{*+}, Z_b^{*+} и Z_a^{*++}, Z_b^{*++} are accordingly, the effective charges of atoms and ions of the first and second degrees of ionization of the interacting particles, respectively.

Most atoms and ions of complex atomic structures feature a built-in and induced dipole electric moment. Therefore, the electron–dipole and dipole–dipole interactions should be taken into account.

Electron-dipole interaction. In the process of the interaction of the atomic particles the built-in dipole electric moments are arranged so that they ensure maximum overlap of the wave functions of the interacting particles with their orbits. In the process of the exchange interaction between the interacting particles, a negative charge *ΔQ* arises; the value of the charge is determined above by formula (15). This negative charge interacts with the dipole moments of the first and second interacting particles, weakening the binary bond between the particles. The energy of this bond is as follows:

$$E_{e-d} = \frac{8\Delta Q}{4\pi\varepsilon_0 r_e^2}\left((1-P_a)p_{э,1} + (1-P_b)p_{э,2} + P_aP_a^+p_{э,3} + P_bP_b^+p_{э,4} + P_aP_a^{++}p_{э,5} + ...\right), \quad (17)$$

where $p_{э,1}$, $p_{э,2}$, $p_{э,3}$, $p_{э,4}$, $p_{э,5}$ и $p_{э,6}$ are the built-in dipole electric moments of ions of the first, second and third ionization of interacting particles. Odd values refer to atom A while even values refer to atom B.

The presence of built-in electric moments in the interacting particles leads to the appearance of a dipole-dipole bond.

Dipole-dipole bond. A dipole-dipole bond in the binary interaction of complex particles is determined according to the following formula:

$$E_{dip.-dip.} = 2[(1-P_a)(1-P_b)\frac{p_{э,1}p_{э,2}}{4\pi\varepsilon_0 r_e^3} + P_a^+ P_b^+ \frac{p_{э,3}^+ p_{э,4}^+}{4\pi\varepsilon_0 r_e^3} + P_a^{++} P_b^{++} \frac{p_{э,5}^{++} p_{э,6}^{++}}{4\pi\varepsilon_0 r_e^3} + ...] \quad (18)$$

In the formation of an ionic bond, a cross interaction of dipole electric moments is formed. Then, taking into account (18)

$$E_{dip.-dip.}^+ = 2\Theta\frac{p_{э,1}p_{э,4}}{4\pi\varepsilon_0 r_e^3} + 2\Theta\frac{p_{э,2}p_{э,3}}{4\pi\varepsilon_0 r_e^3}. \quad (19)$$

In the process of the binary interaction, a particle with shared electron shell is formed due to sharing of outer electrons. The bond breaking energy for a newly formed particle is determined by all types of bonds combined. In this case, it is essential to know the effective radiuses of the interacting particles and the equilibrium distances between them. The interaction potential, even considered with taking into account all the above interactions at close distances, does not make it possible to obtain a significant decrease in the binding energies (D_e). In this regard, let us consider the process of the interaction of the ions of a positive core, which quite effectively reduces the binding energy of the interacting atoms in a diatomic molecule.

Coulomb repulsion of the particles of a positively charged ionic core

In complex molecular systems, the valence electrons of individual atoms are shared, and a condensed medium appears in the form of a two-component mixture consisting of a generalized electron cloud and an ionic core of single ions. The electrons of neutral atoms are bound to a positively charged core with their effective charge. These effective charges interact with each other when they open due to the overlap of their wave functions. Based on the divergence theorem, the flux of the electric displacement vector is equal to the charge inside a closed surface. In the presence of a second positive charge, the flux of the electric displacement vector is deformed and a third one - negative charge - arises on the surface that separates two positive charges. The electric displacement vector is directed perpendicular to the surface.

Then the flux of the electric displacement vector through this surface amounts to:

$$N_{a,(b)} = \int_0^{\pi r_0^2} \frac{z^* e \cos(\alpha)}{4\pi r_{a,(b)}^2} dS \,, \tag{20}$$

where z^* is the effective charge of a positive ion, $dS = 2\pi r dr$ and $r_0 = \sqrt{r_{a,(b)}^2 - (r_e / 2)^2}$, $\alpha = \arctan\left(\frac{2r}{r_e}\right)$.

Accordingly, the share of the charge involved in the mutual repulsion is:

$$\xi_{a,(b)} = N_{a,(b)} / Z^* e \,. \tag{21}$$

In addition, the mutual screening of the effective charge should be taken into account since each successive ion charge is screened by the previous energy levels of the atomic system, i.e.:

$$Z_{a,k}^* = Z_{a,k} - Z_{a,k-1} - Z_{a,k-2} - \ldots$$

Then the repulsion energy amounts to:

$$U_a = P_a P_b \frac{\xi_a \xi_b Z_a^* Z_b^*) e^2}{4\pi\varepsilon_0 r_e} + P_a^+ P_b^+ \frac{\xi_a^+ \xi_b^+ Z_a^{*+} Z_b^{*+} e^2}{4\pi\varepsilon_0 r_e} + P_a^{++} P_b^{++} \frac{\xi_a^{++} \xi_b^{++} Z_a^{*++} Z_b^{*++} e^2}{4\pi\varepsilon_0 r_e} + \ldots \tag{22}$$

When negative ions are formed, a repulsion arises between the induced charge and the external electron of the negative ion, i.e.

$$E = \frac{\Delta Q e}{4\pi\varepsilon_0}\left(\frac{1}{r_1} + \frac{1}{r_2}\right). \tag{23}$$

Therefore, positive ions inhibit the exchange of electrons within the ionic core, and this is precisely what is taken into account in the Heitler-London theory. In addition, they mutually repel according to Coulomb's law. Each valence electron can be, with a certain probability, in the region of overlapping wave functions of neutral atoms and positive ions inside the core. In this case, based on the principle of superposition of electric fields, it is necessary to take into account the interaction of each ion with all other ions inside the positive core of the molecule. Specifically, for the binary interaction, this situation is shown in Figure 2.

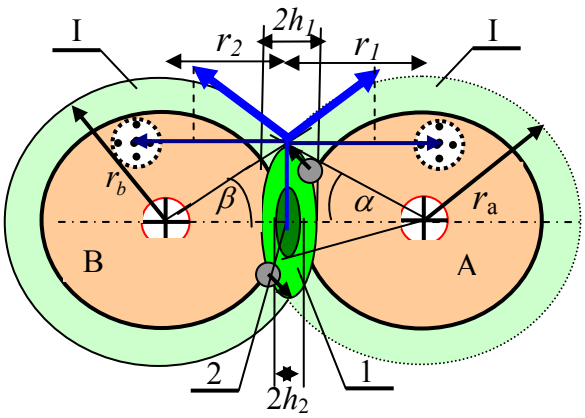

Figure 2 – Coulomb interaction of nuclei in the binary interaction of atoms
Рис. 2 – Кулоновское взаимодействие ядер в бинарном взаимодействии атомов
Слика 2 – Кулонова интеракција нуклеуса у бинарној интеракцији атома

The overlap zone for the valence electron of the neutral atom A is formed by the angle α while the one for the atom B is formed by the angle β; these angles are determined by formulas (11) and (12). The overlap zone of the wave functions of the single ionization is indicated by the number 1, and the overlap zone of the wave functions of the double ionization is indicated by the number 2.

The interaction energy of the positive ions of the core amounts to:

$$U_{res.}^{+} = \sum_i P_i^{+} \frac{Z_i^2 e^2}{4\pi\varepsilon_0 r_e} . \tag{24}$$

Thus, the total energy of the interaction of atoms in a diatomic molecule is realized as the following sum:

$$E_{res.} = E_{\text{cov.}} + E_{ion} + E_{ind.} + E_{el.-dip.} + E_{dip.-dip.} + U_{res.}^{+} . \tag{25}$$

Thus, the interaction potential of atoms in a diatomic molecule is determined as such a complex aggregate. Below the interaction potentials for some diatomic molecules were calculated in comparison with the Lennard-Jones and Morse potentials as an example.

Interaction potentials of the diatomic molecules and their analysis

The calculations of the interaction potentials have been performed under the following restrictions:

1. At the internuclear distance of $r_e = r_a + r_b$ and farther, only the exchange interaction occurs, the repulsion of the ions of the positive core is sharply weakened while the interaction of the built-in electric dipoles occurs only for neutral atoms.

2. For distances at which the overlap integral *S* is greater than unity, the ionic, induced, and electron-dipole bonds are equal to zero.

3. At all internuclear distances, the bond exchange energy is always greater than the dipole-dipole bond.

4. The overlap integral is always less than one.

Specific calculations of the interaction potentials have been performed for diatomic molecules of carbon, nitrogen, oxygen, silicon, aluminum and sodium, for which the dissociation energy varies from a maximum value of 9.76 eV to a minimum value of 0.76 eV and they are shown in Figures 3 to 8. This is enough to fully understand the dynamics of the formation of interaction potentials during the formation of diatomic molecules.

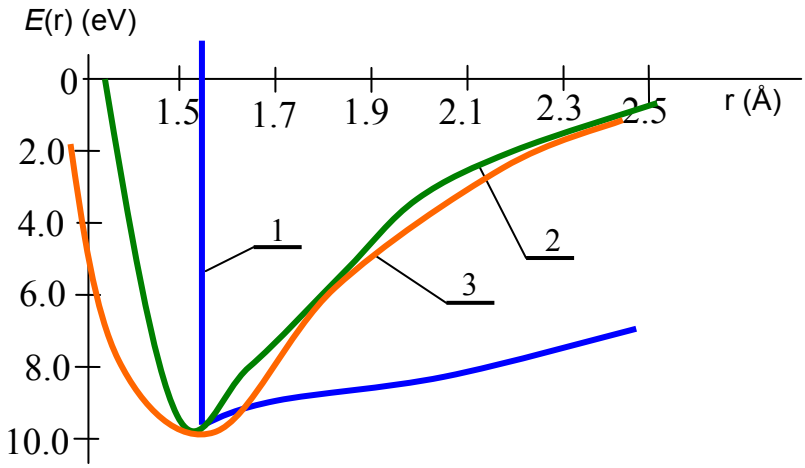

Figure 3 – Interaction potential in the diatomic nitrogen molecule obtained using: 1 - formula (25); 2 - Lennard-Jones formula; 3 - Morse formula

Рис. 3 – Потенциал в двухатомной молекуле азота полученный по формуле: 1 - (25); 2 - Леннарда-Джонса; 3 - Морзе

Слика 3 – Потенцијал интеракције у двоатомском молекулу водоника добијен помоћу: 1 - формуле 25, 2 - Ленард-Џонсове формуле, 3 - Морзеове формуле

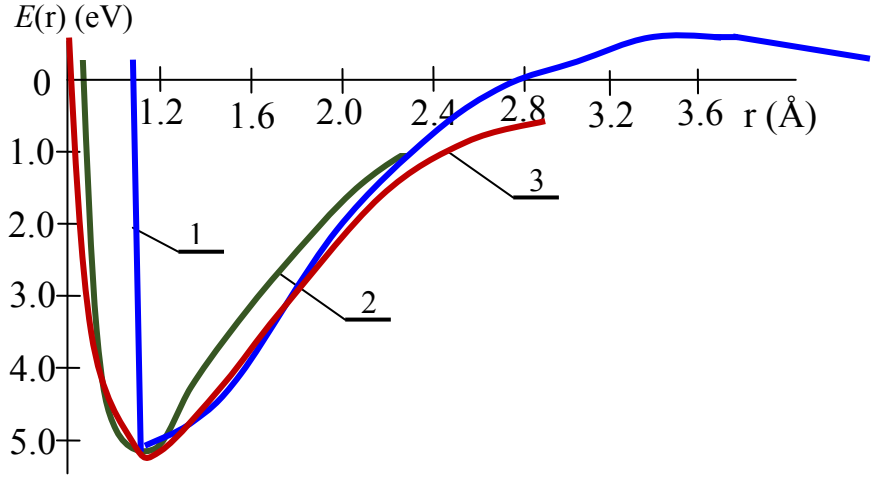

Figure 4 – Interaction potential in the diatomic oxygen molecule calculated using: 1 - formula (25); 2 - Lennard-Jones formula; 3 - Morse formula

Рис. 4 – Потенциал в двухатомной молекуле кислорода полученный по формуле: 1 - (25); 2 - Леннарда-Джонса; 3 - Морзе

Слика 4 – Потенцијал интеракције у двоатомском молекулу кисеоника добијен помоћу: 1 - формуле 25, 2 - Ленард-Џонсове формуле, 3 - Морзеове формуле

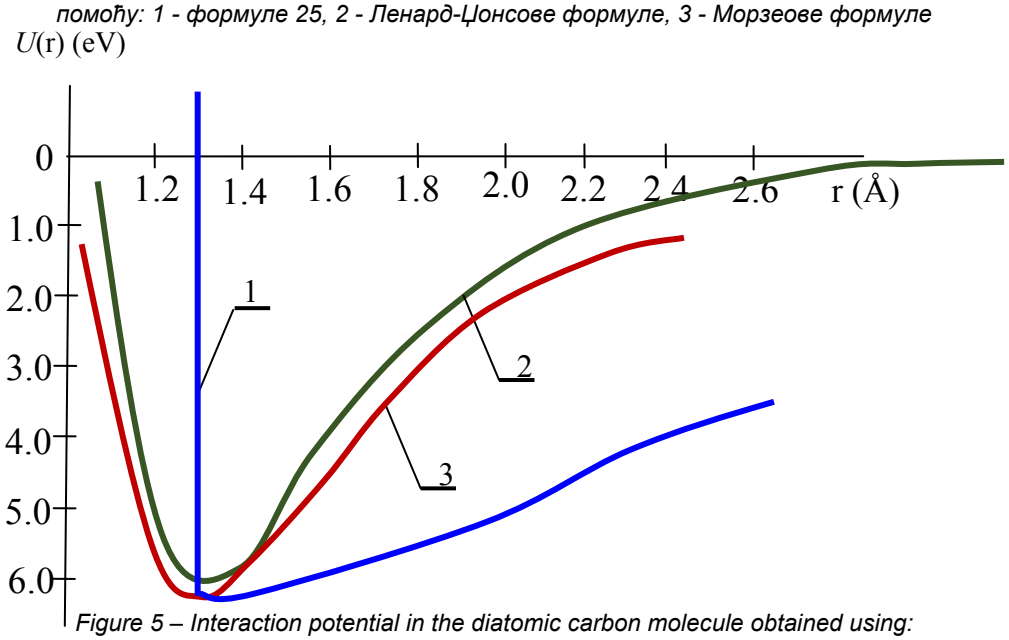

Figure 5 – Interaction potential in the diatomic carbon molecule obtained using: 1 - formula (25); 2 - Lennard-Jones formula; 3 - Morse formula

Рис. 5 – Потенциал взаимодействия в двухатомной углерода полученный по формуле: 1 - (25); 2 - Леннарда-Джонса; 3 - Морзе

Слика 5 – Потенцијал интеракције у двоатомском молекулу угљеника добијен помоћу: 1 - формуле 25, 2 - Ленард-Џонсове формуле, 3 - Морзеове формуле

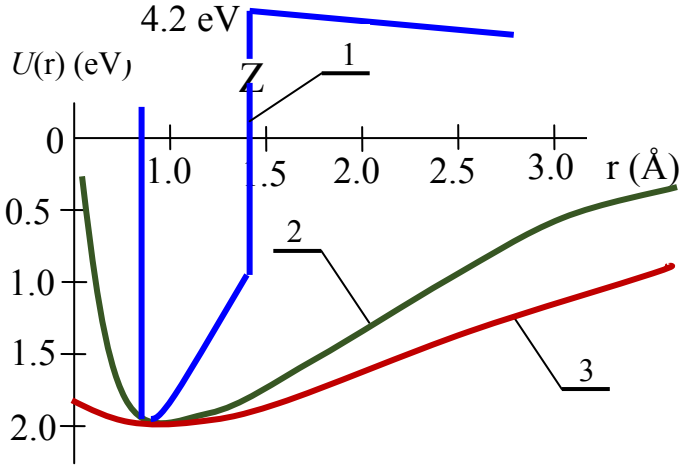

Figure 6 – Interaction potential in the diatomic aluminum molecule obtained using: 1 - formula (25); 2 - Lennard-Jones formula; 3 - Morse formula
Рис. 6 – Потенциал взаимодействия в двухатомной молекуле алюминия полученный по формуле: 1 - (25); 2 - Леннарда-Джонса; 3 - Морза
Слика 6 – Потенцијал интеракције у двоатомском молекулу алуминијума добијен помоћу: 1 - формуле 25, 2- Ленард-Џонсове формуле, 3 - Морзеове формуле

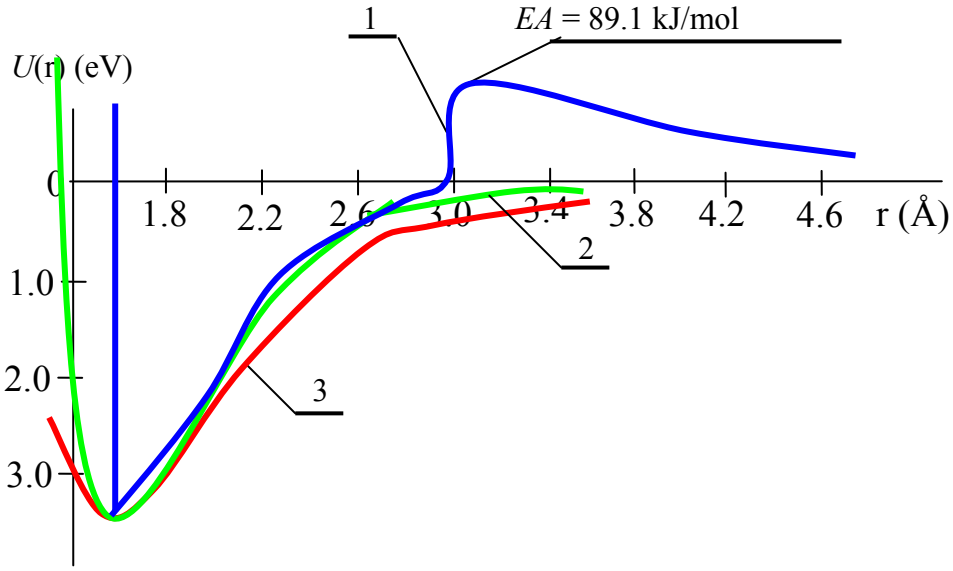

Figure 7 – Iinteraction potential in the diatomic silicon molecule obtained using: 1 - formula (25); 2 - Lennard-Jones formula; 3 - Morse formula
Рис. 7 – Потенциал взаимодействия в двухатомной молекуле кремния полученный по формуле: 1 - (25); 2 - Леннарда-Джонса; 3 - Морза
Слика 7 – Потенцијал интеракције у двоатомском молекулу силицијума добијен помоћу: 1 - формуле 25, 2 - Ленард-Џонсове формуле, 3 - Морзеове формуле

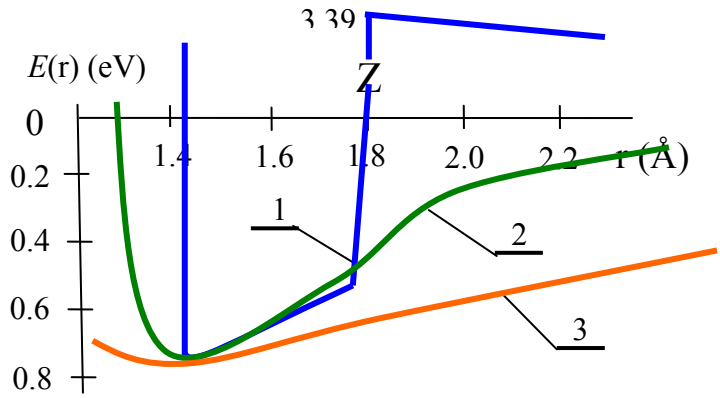

Figure 8 – Interaction potential in the diatomic sodium molecule obtained using: 1 - formula (25); 2 - Lennard-Jones formula; 3 - Morse formula
Рис. 8 – Потенциал взаимодействия в двухатомной молекуле натрия полученный по формуле: 1 - (25); 2 - Леннарда-Джонса; 3 - Морза
Слика 8 – Потенцијал интеракције у двоатомском молекулу натријума добијен помоћу: 1 - формуле 25, 2 - Ленард-Џонсове формуле, 3 - Морзеове формуле

Table 2 – Radii of atoms and the values of different binding energies in the energy of dissociation
Таблица 2 – Радиусы атомов и значения разных энергий связи в энергии диссоциации
Табела 2 – Пречници атома и вредности различитих везивних енергија у енергији дисоцијације

Mo-lec.	The calculated atomic radii and internuclear distances as well as the values of different interaction energies in eV								
	r_a (Å)	r_e (Å)	$E_{cov.}$	E_{ion}	$E_{ind.}$	$E_{el.-dip.}$	$E_{dip-dip.}$	$E_{разл.}$	D_e
N_2	1.109 0.746	1.3974/1.098 1.0696	-7.402 -2.464	-1.533 -1.873	-1.613 -0.778	0.102 0.070	0.111 0.096	0.575 0.119	9.760/9.76 4.829
C_2	1.201	1.2896/1.242	-4.450	-1.010	-3.007	0.360	0.510	1.476	6.200/6.2
O_2	0.8675 0.74 0.672	1.189 /1.207 1.07 0.992	-3.304 -2.404 -1.983	-1.720 -1.804 -1.897	-1.023 -0.791 -0.714	-0.104 -0.086 -0.052	0.545 0.408 0.169	0.487 0.235 0.152	5.120/5.12 4.370 4.053
Si_2	1.502 1.56	1.985/2.246 2.035	-1.561 -1.330	-0.255 -0.190	-2.132 -2.346	0.002 0.003	-0.038 -0.037	0.581 0.654	3.400/3.4 3.247
Al_2	0.718	1.096/2.56	-0.736	-0.863	-815	0.110	0.052	0.253	2.00/2.0
Na_2	0.8867	1.4565/3.077	-.404	-.230	-0.290	0	0	0.174	- 0.750

An important property of the interaction potentials is that for given ionization potentials and dipole electric moments, the experimental value of the dissociation energy is realized with a strict ratio of the effective energy radius of a neutral atom and the distance between nuclei in a diatomic molecule. In this case, the effective energy radius should not coincide with the radius of the atom, since the radius of the atom corresponds to the maximum of the electron density distribution function while the effective energy radius of the interaction is determined by the mutual compensation of the positive and negative binding energies at an equilibrium distance. Predominantly, the energy radius turned out to be greater than the radius of the atom obtained by calculations using the Hartree-Fock wave functions (Brattsev, 1966). Only for silicon, the energy radius turned out to be ~ 10% less while for sodium both radii completely coincided.

For most diatomic molecules, the calculated equilibrium distance between atoms turned out to be greater than the equilibrium distance obtained from the vibrational spectra. Only for silicon and sodium did these values turn out to be less than the equilibrium distance obtained from the vibrational spectra.

The specific calculated values of the energy radii and the equilibrium distances of the interacting atoms as well as the values of different binding energies in diatomic molecules are summarized in Table 2.

The internuclear distance for all molecules does not coincide with the values obtained from the vibrational spectra. These values in Table 2 are shown after slash.

The induced binding energy, which was substantiated in the work (Gretchikhin et al, 2015, pp.29-41), and the repulsion energy introduced in this article, turned out to be determining. Without taking them into account, the interaction potential in diatomic molecules cannot be determined.

Average effective radius of molecules and ionization energy of binary formations

In diatomic molecules, the valence electrons travel each around their atoms. When both electrons enter the overlap zone, an exchange of electrons occurs. The bond of one of the external electrons with the core of the molecule determines the ionization potential while the second electron screens the core of the molecule. Obviously, such screening should be different depending on the size and structure of the electron shells of the interacting atoms. Each of the external valence electrons in

the diatomic molecule interacts with one of the nearest atomic nuclei in two positions shown in Figure 2. Thus, the effective radius of the molecule can be represented as follows:

$$r_m = [(r_a + r_1) + (r_b + r_2) + \sqrt{r_a^2 - r_1^2} + \sqrt{r_b^2 - r_2^2}]/4 \qquad (26)$$

The probability of electrons being in the overlap zone is determined by formulas (11) and (12) while taking into account the fact that they do not exchange their states. Accordingly, for each electron, the resulting probability of staying in the overlap zone is $P_a(1-S)$ и $P_b(1-S)$.

Outside the overlap zone, the ionization energy of the atom A is equal to the single ionization of the atom A. In the overlap zone, if the electron does not transfer from the atom A to the atom B, the ionization energy still corresponds to the atom A. The electron in the atom A is either in the overlap zone or outside this zone. The resulting probability of this event for the atom A, taking into account the fact that the valence electron is located at a distance of r_1 from the nucleus of the atom, is equal to [(1-P_a) + $P_a(1-S)r_a/r_1$] while the probability for the atom B is equal to [(1-P_b) + $P_b(1-S)r_b/r_2$]. Then, for the electron near the atom A, the ionization energy of the molecule will amount to:

$$IP_a = [(1-P_a) - P_a(1-S)r_a/r_1]\theta_a + P_a(1-)\theta_b - P_a\frac{dqe}{4\pi\varepsilon_0 r_1)}, \qquad (27)$$

while that for the electron near the atom B will amount to:

$$IP_b = [(1-P_b) + P_b(1-S)r_b/r_2]\theta_b + (1-P_b)P_a\theta_a - P_b\frac{dqe}{4\pi\varepsilon_0 r_2)}. \qquad (28)$$

Here θ_a and θ_b are the ionization energies of the atom A and the atom B, respectively.

The results of the calculations of the ionization energies and the radii of neutral molecules and their ions of the first as well as the second multiplicity of ionization of some diatomic molecules are presented in Table. 3 as an example. The reference data for the first multiplicity of ionization of some diatomic molecules is shown in Table 3 after slash.

Agreement with the data for diatomic molecules, given in the handbook (Radzig & Smirnov, 1985), for the energies of single ionization, is quite satisfactory. A number of molecules feature a relatively large dipole electric moment. This property of molecules is still not clear. When the molecules in which the initial atoms have a built-in dipole electric moment are considered, this property of molecules can be understood.

However, even in the case of simple diatomic molecules, such as BH and LiH, in which the initial atoms do not have a built-in dipole electric moment, their own dipole electric moments are quite substantial. This property of molecules needs further justification.

Table 3 – Ionization energy of diatomic molecules of the single and double ionization multiplicity

Таблица 3 – Энергия ионизации двухатомных молекул первой и второй кратности ионизации

Табела 3 – Јонизациона енергија двоатомских молекула једноструке и двоструке мултипликативности јонизације

Parameters	Molecules					
	C_2	N_2	O_2	Al_2	Si_2	Na2
$r_{m,1}$ (Å)	1.410	1.550	1.067	2.129	1.811	1.060
Z_1^*	1.173	1.618	0.909	0.964	0.954	0.361
Θ_1 (eV)	11.87/ 11.9	15.05/ 15.58	12.515/ 12.077	6.527 -	7.596/ 7.4	4.916/ 4.9
$r_{m,2}$ (Å)	0.953	0.965	0.756	1.488	1.277	0.908
Z_2^*	2.173	2.618	1.909	1.964	1.954	1.361
Θ_2 (eV)	32.87	39.11	36.40	19.026	22.057	21.6

In order to exclude the influence of intrinsic built-in dipole electric moments of the initial atoms, let us consider, as an example, the aforementioned simple diatomic molecules BH LiH. For these molecules, the dipole electric moments are respectively 4.33·10-30 C·m and 19.6·10-30 C·m (Radzig & Smirnov, 1985). The first value was obtained with an error exceeding 10% while the second one - with an error not exceeding 1%, i.e., quite accurately.

The calculation of the dissociation energies of these molecules is presented in Table 4.

Table 4 – Values of the binding energies of diatomic molecules from different atoms without built-in dipole electric moments

Таблица 4 – Величина энергий связи двухатомных молекул из разных атомов без встроенных дипольных электрических моментов

Табела 4 – Вредности везивних енергија двоатомских молекула састављених од различитих атома без уграђених електричних диполних момената

Mo-lec.	r_a (Å)	Values of different binding energies (eV)						r_e (Å)	$p_{e,m}$ $\cdot 10^{-30}$
		$E_{cov.}$	E_{ion}	$E_{exch.}$	$E_{res.}(D_0)$	IP (eV)	r_m (Å)		
B+H	1.16	-1.854	-1.306	-0.241	3.39	11.06	1.010	1.290	11.64/ 4.43
Li+H	1.68	-0.548	-0.835	-1.047	2.429	8.81/ 7.78	1.238	1.688	18.39 19.6
O+H	0.67	-3.529	-0.702	-0.123	4.40	12.91	0.942	1.510	

The dissociation energy and the internuclear distance for the HV molecule are obtained from the equality of the theoretical value of the dissociation energy obtained experimentally with an error not exceeding 10%, which is quite an acceptable value. Therefore, the obtained value of the dipole electric moment by theoretical calculation presents quite a realistic value. The probability of the presence of both valence electrons near the atom of boron and hydrogen is 0.483 and 0.104, respectively.

For the LiH molecule, the situation is rather complicated since the radius of the lithium atom needs to be clarified. If the radius of the lithium atom calculated using the modified Slater wave functions and given in the handbook (Radzig & Smirnov, 1985) is used, then the minimum potential energy of the interaction between lithium and hydrogen atoms is realized at a distance between atoms of $r_e = 2.5$ Å while the interaction energy amounts only to $D_0 = 1.422$ eV. To obtain, by calculations, an experimental value equal to 2.429 eV, it is necessary to assume that $r_e = 1.688$ Å and the radius of lithium atom $r_a = 1.68$ Å but not $r_a = 2.049$ Å (Radzig & Smirnov, 1985), (Slater, 1937). The probability of the presence of both valence electrons near the atoms of lithium and hydrogen is 0.640 and 0.040. Therefore, both for the HV molecule and for the LiH molecule, the boron and lithium atoms with respect to the hydrogen atom are more negative, which determines such a large value of the dipole electric moment of these molecules. For other molecules the situation is similar.

Thus, the interaction of atoms in a diatomic molecule is a rather complicated process, in which the exchange interaction of electrons of the single ionization of the interacting atoms should be taken into account, as well as the presence of built-in electric moments of the atoms that are directed inside the molecule relative to each other as well as the probability of stay of valence electrons relative to the interacting atoms. It should be specially noted that the positively charged nuclei of the interacting atoms impede the exchange of valence electrons and, in turn, repel each other according to Coulomb's law.

Conclusions

As a result of the studies of different types of chemical bonds between atoms, it was found:

1. The following types of interactions have been clarified: exchange, ionic, induced, electron-dipole, dipole-dipole and nuclear repulsion energies, and the probability of their occurrence has been determined.

2. The covalent bond is not decisive and is due only to the exchange of valence electrons of neutral atoms.

3. It is shown that the probability of valence electrons staying in the overlapping region of wave functions can be determined not only by the residence time of valence electrons near interacting atoms but also by the ratio of the area of the overlapping wave functions to the entire area of the sphere on which the electron travels.

4. A theory of the interaction of atomic nuclei in a diatomic molecule of identical atoms has been developed.

5. The interaction potentials for a number of diatomic molecules have been calculated in comparison with the Lennard-Jones and Morse potentials and the failure of empirical interaction potentials has been shown.

6. At the double energy radius of the molecules, a potential jump occurs with a transition from the negative to the positive region of binding energies and determines the activation energy of the formation of diatomic molecules.

7. The obtained atomic radii and the internuclear distances of diatomic molecules are effective values at which the experimental values of the binding energies are realized.

The development of various theories of chemical bonds, taking into account their probabilities of occurrence, is at the initial stage of their formation.

It seems possible, based on the obtained interaction potentials of atoms in diatomic molecules, to determine the activation energy, ionization energy, standard atomization enthalpy, and electron affinity for diatomic molecules. A lot of scientific work is ahead in this direction.

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МЕЖАТОМНОЕ ВЗАИМОДЕЙСТВИЕ В ДВУХАТОМНЫХ МОЛЕКУЛАХ С УЧЕТОМ РАСТАЛКИВАНИЯ ИОНОВ В ПОЛОЖИТЕЛЬНОМ ОСТОВЕ

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Резюме:

Введение/цель: Проведен анализ разных типов взаимодействий в двухатомных молекулах из сложных атомов.

Методы: Для учета сил отталкивания и притяжения в молекуле используются эмпирические формулы Леннарда-Джонса, Бакингема, Бакингема-Корнера, Морзе, Данема, Гульберта-Гиршфельдера, Клейна и их комбинации без четкого физического обоснования. Улучшить ситуацию бинарного взаимодействия внутри конденсированных сред Гречихин и сотрудники предложили применить квантовую теорию Гайтлера-Лондона, но только на расстояниях больше равновесного. При расстояниях менее равновесного между атомами в бинарном взаимодействии по-прежнему использовалась формула Леннарда – Джонса. Применяя разного рода подгоночные коэффициенты, в каждом конкретном случае получали совпадение с экспериментальными данными по энергии диссоциации. Более общее представление о всех возможных типах взаимодействий полностью отсутствовало. В этой связи возникла необходимость выявить все возможные типы взаимодействий внутри двухатомных молекулах и теоретически получить энергию диссоциации, энергию активации, стандартную энтальпию атомизации. Применение методов квантовой механики позволило в теории Гайтлера-Лондона учесть не только кулоновское сдерживание при обменном взаимодействии, но и кулоновское отталкивание ядер.

Результаты: Проведен расчет электрических диполей у нейтральных атомов и у положительно заряженных ионов остова двухатомных молекул. Это позволило произвести расчет электрон-дипольного и диполь-дипольного взаимодействия. Разработана теория отталкивания положительно заряженных ядер сложных атомов в двухатомных молекулах. Выполнен расчет потенциалов взаимодействия для молекул углерода, азота, кислорода, алюминия, кремния и натрия. Проведено сравнение разработанной физической модели формирования двухатомных молекул с эмпирическими потенциалами Леннарда-Джонса и Морзе. На межъядерном расстоянии, равном сумме энергетических радиусов атомов в молекуле происходит скачок потенциала с переходом из отрицательной в положительную область энергий связи, что определяет энергию активации образования двухатомных молекул.

Выводы: Из полученных потенциалов взаимодействия атомов в двухатомных молекулах определены энергия активации,

энергия ионизации, стандартная энтальпия атомизации и сродство к электрону.

Ключевые слова: потенциал взаимодействия, ковалентная связь, ионная связь, электрический диполь, наведенная связь, двухатомная молекула.

ИНТЕРАКЦИЈА ИЗМЕЂУ АТОМА У ДВОАТОМСКИМ МОЛЕКУЛИМА ПРИ ОДБИЈАЊУ ЈОНА У ПОЗИТИВНО НАБИЈЕНОМ ЈЕЗГРУ

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Сажетак:

Увод/циљ: Анализирају се различити облици интеракција у двоатомским молекулима сложених атома.

Методе: Користе се емпиријске формуле Ленард-Џонса, Бакингема, Бакингем-Корнера, Морзеа, Данема, Гилберт-Хиршфелдера, Клајна, као и њихове комбинације без јасне реалне оправданости, при анализи одбојних и привлачних сила у молекулу. За побољшање ситуације бинарне интеракције унутар згуснуте материје, Гречихин и његови сарадници су предложили примену квантне теорије Хајтлера и Лондона, али само за раздаљине веће од равнотежног стања. Ленард-Џонсова формула била је коришћена и на раздаљинама мањим од равнотежног стања између атома у бинарним интеракцијама. У сваком случају постигли смо поклапање са експерименталним подацима о дисоцијацији енергије користећи различите врсте одговарајућих коефицијената. Уопштенија идеја о свим могућим типовима интеракција потпуно је изостала. С тим у вези, било је потребно открити све могуће типове интеракција унутар двоатомских молекула и теоретски добити енергију дисоцијације, енергију активације и стандардну енталпију атомизације. Примена метода квантне механике у Хајтлер-Лондоновој теорији омогућила је да се узме у обзир не само Кулоново одбијање током интеракције размене већ и Кулоново одбијање нуклеуса.

Резултати: Израчунати су електрични диполи за неутралне атоме и за позитивно наелектрисане јоне језгара двоатомских молекула, што је омогућило израчунавање електрон-дипол интеракција, као и дипол-дипол интеракција. Развијена је теорија

одбијања позитивно наелектрисаних нуклеуса сложених атома у двоатомским молекулима. Израчунати су потенцијали за молекуле угљеника, алуминијума, силицијума и натријума. Развијени физички модел формирања двоатомских молекула упоређен је са емпиријским потенцијалима Ленард-Џонса и Морзеа. На раздаљини између нуклеуса, једнакој збиру енергија пречника атома, у молекулу долази до скока потенцијала с прелазом од негативне до позитивне области енергије везивања, што детерминише активациону енергију формирања двоатомских молекула.

Закључак: Из добијених потенцијала интеракција атома у двоатомским молекулима одређени су енергија активације, енергија јонизације, стандардна енталпија атомизације, као и афинитет према електрону.

Кључне речи: потенцијал интеракције, ковалентна веза, јонска веза, електрични дипол, индукована веза, двоатомски молекул.

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