

## Concept of electrons pairing during the formation of covalent chemical bonds

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### Abstract

This research studies the forces acting in an electron pair with antiparallel spins participating in forming a covalent chemical bond between atoms. The first is the force of electrostatic repulsion of electrons. The second is the gravitational attraction of these electrons. The third is the force of electromagnetic attraction between the electron pair. From calculations it follows, that the force of gravitational attraction is negligible, and therefore it is not able to withstand the force of electrostatic repulsion between electrons. However, the force of electromagnetic attraction between a pair of electrons with antiparallel spins turned out to be hundreds of times greater than the force of their electrostatic repulsion. As a result, the formation of stable electron pairs in molecular orbitals becomes possible. Thus, valence electrons of neighboring atoms interact with each other like femto-electromagnets, as a result of which a stable bond is formed between these electrons. Calculations have shown that in hydrogen molecule the force of electrostatic attraction between nuclei and paired electrons of a molecular orbital significantly exceeds the force of electrostatic repulsion of nuclei, which ensures the formation of a strong covalent chemical bond. To form covalent bonds in other molecules, the force of electrostatic attraction between the nuclei and paired electrons of the molecular orbitals must be much greater than the forces of electrostatic repulsion between both the positively charged nuclei and the negatively charged electrons of the atomic orbitals of different atoms.

**Keywords:** Covalent bonds; Electrons; Pairing of electrons; Spin of electrons; Electrostatic force; Gravitation force; Electromagnetic force

### 1. Introduction

As is known, matter consists of atoms and ions, which can bind to each other and form simple and complex structures and molecules [1]. An example of atomic structure is the structure of some simple substances such as helium, argon, neon, etc. Under normal conditions, these substances are inert gases, but after cooling, they form liquids and crystals consisting of atoms of the corresponding simple substance, connected by weak interatomic van-der-Waals bonds of a dispersion nature.

Ions can form metallic and ionic bonds. Metals have crystal lattices, in the nodes of which positive ions (cations) of the metals are located bonding electrons with the Coulomb attraction force [2, 3]. Such a metallic bond arises because metal atoms easily lose their outer, weakly bound electrons and become cations, while the electrons become shared and interact with many cations. Common electrons of metals move randomly between the cations and connect them with Coulomb force, thereby preventing the disintegration of the metal lattice under the action of repulsive forces of positive cations.

An ionic bond is a type of electrostatic interaction between atoms having a large electronegativity difference over 1.7 [4]. For the ionic bond to be formed, the more electronegative atom must have vacancies in the outer orbital, causing the electrons with higher energy belonging to the less electronegative atom to jump and occupy these vacancies. This

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bonding type usually exists in ionic crystals consisting of cations and anions. A typical example of such crystals is sodium chloride, in which the halogen captures the outer valence electron of the alkali metal and turns it into an anion with a stable 8-electron shell. On the other hand, the alkali metal loses a valence electron and turns into a cation, also with a stable 8-electron shell. Thus, chemical bonding in ionic crystals is realized due to the Coulomb interaction between the oppositely charged ions that form the crystal lattice.

More difficult is to explain the mechanism of the formation of covalent non-polar and polar chemical bonds between atoms in molecules. It is generally believed that a covalent bond between atoms in a molecule is formed by the inclusion of valence electrons of atoms into the molecular orbital to form a shared electron pair with antiparallel spins [2, 5]. It is also known that electrons of various outer orbitals in atoms (s, p, etc., as well as hybrid orbitals) can participate in the formation of these chemical bonds.

Molecules containing identical atoms have non-polar covalent bonds, where the shared electron pair belongs equally to both atoms of the molecule. The simplest example is the formation of a hydrogen molecule from two atoms of this element by pairing the valence electrons of neighboring atoms. According to the theory of molecular orbitals, two outer s-orbitals of hydrogen atoms form two molecular orbitals, bonding and antibonding. Moreover, a pair of shared valence electrons of atoms are located in the lower-energy bonding orbital. On the other hand, the theory of valence bonds explains the formation of a covalent bond in a hydrogen molecule by the overlapping of the outer s-electron orbitals of the atoms.

A non-polar covalent bond does not necessarily require that the two atoms be of the same; it is enough that they have close electronegativity. However, in polar molecules with a significant difference in the electronegativity of atoms up to 1.7, the common electron pair is shifted towards the more electronegative atom.

For quantum mechanical calculations of covalent bonding, two main theories have been proposed, such as molecular orbitals (MO) and valence bonds (VB) [6, 7]. According to the MO theory, molecular orbitals are formed by combining atomic orbitals. As a result, three types of molecular orbitals appear, such as bonding, antibonding, and non-bonding. Electrons in bonding molecular orbital strengthen the bond, while in antibonding orbital destabilize it. Electrons in non-bonding molecular orbitals do not participate in the formation of a chemical bond. MO theory postulates that a molecule will be stable only if the number of electrons in bonding orbitals exceeds the number of electrons in antibonding ones. Thus, the concept of covalent bonding in MO theory is rather vague.

Unlike the MO theory, the VB theory provides a clearer definition of chemical bonds. According to the VB concept, a covalent bond is achieved as a result of the overlapping of outer electron orbitals of atoms and the pairing of the spins of electrons located in these orbitals. As a result of bonding into a molecule, the energy of atoms decreases. The strength of a covalent bond in a molecule depends on the degree of overlapping of the outer orbitals of atoms.

Some textbooks describe an additional qualitative concept, according to which the valence electrons of neighboring atoms are considered waves. When these waves interfere in one phase, they will be amplified, which is interpreted as the formation of a chemical bond. However, an increase in amplitude means an increase in energy, which contradicts the theory, according to which after bonding, the energy of atoms should decrease. From this point of view, to form a covalent chemical bond with the lowest energy, electron waves must interfere in an antiphase, which is similar to the formation of a pair of electrons with antiparallel spins.

In studying the nature of covalent bonding, an unsolved problem arises, which is that regardless of the proposed theories and qualitative concepts of the covalent bond, the scientific literature does not explain how such a bond can be formed at all if two negatively charged electrons in a pair must repulse each other, and not bond. For example, it is unclear how repulsive electrons can form a bonding molecular orbital (in MO theory) or why the overlapping of electron orbitals (clouds) of neighboring atoms occurs instead of their repulsion (in VB theory)

This study aimed to analyze the various forces that can prevent the electrostatic repulsion of electrons and allow them to form stable pairs with antiparallel spins in molecular orbitals. In addition, the formation mechanism of covalent bonds was investigated.

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## 2. Results and Discussion

It should be noted that here the equations of classical physics were used for the calculations, which gave only approximate results but allowed us to trace the trends in the directions of action and magnitudes of the forces at the femto-pico meter levels. This was done to simplify and speed up the calculations. In addition, calculations performed

using the equations of quantum physics for MO and VB theories are not always sufficiently reliable [7], so we abandoned their use in this study.

Let's consider what forces can act in an electron pair. First of all, this is the Coulomb repulsion force ( $F_{r,c}$ ) between negatively charged electrons having charge  $e$ . The second force ( $F_{a,g}$ ) is caused by the gravitational attraction of electrons with mass  $m_e$ . In addition, it is well known that due to the spin, the electron has a magnetic moment  $\mu_s$ , the absolute value of which is very close to the value of the Bohr magneton  $\mu_b$ :

$$\mu_s \approx \mu_b \quad (1)$$

The presence of a magnetic field caused by the quasi-circular rotation of electrons called spin can lead to the emergence of an attraction electromagnetic force ( $F_{a,em}$ ) between the electron pair with opposite spins.

For further analysis, it is necessary to quantify these forces. Let two electrons be at a minimum distance ( $L$ ) from each other equal to two effective classical quantum radii ( $r_e$ ) of the electron,  $L = 2r_e = 5.64 \times 10^{-15}$  (m). Then the force of Coulomb repulsion between two electrons can be calculated using the well-known equation:

$$F_{r,c} = 0.25 k (e/r_e)^2 \quad (2)$$

where the constant  $k = 8.99 \times 10^9$  (N m<sup>2</sup>/C<sup>2</sup>), and the electron charge  $e = 1.6 \times 10^{-19}$  (C).

Substituting all the constants, it can be obtained that  $F_{r,c} = 7.24$  N.

The second force of the gravitational attraction between two electrons with mass  $m_e$  was calculated as follows:

$$F_{a,g} = 0.25 G (m_e/r_e)^2 \quad (3)$$

where the gravitation constant  $G = 6.67 \times 10^{-11}$  (N m<sup>2</sup>/kg<sup>2</sup>), and the mass of the electron  $m_e = 9.11 \times 10^{-31}$  (kg).

According to calculations,  $F_{a,g} = 1.74 \times 10^{-42}$  N. Since the force of gravitational attraction is negligible, it is not able to withstand the force of Coulomb repulsion between two electrons.

Therefore, the main attention should be paid to the third force,  $F_{a,em}$ , caused by the electromagnetic attraction of electrons with antiparallel spins to each other. In this approach, such electrons can be considered as femto-sized electromagnets. To estimate the magnitude of electromagnetic force, the following equation was used [8]:

$$F_{a,em} = 1.5 \mu_0 \mu_b I L r_e^2 / (r_e^2 + L^2)^{5/2} \quad (4)$$

where  $L = 2r_e$ ;  $\mu_0 = 4\pi \times 10^{-7}$  (N/A<sup>2</sup>) is the constant of magnetic permeability in a vacuum;  $\mu_b = 9.274 \times 10^{-24}$  (J/T) is the Bohr magneton, while  $I$  is the amperage of quasi-rotating electrons that can be calculated as follows:  $I = 2e c / r_e$ .

After introducing all the constants into eq. (4), it was found that the force of electromagnetic attraction between two paired electrons with opposite spins will be:  $F_{a,em} = 2670$  N.

Since the value of  $F_{a,em}$  is hundreds of times greater than the force of Coulomb repulsion between electrons  $F_{r,c}$ , the above estimate can serve as a convincing argument in favor of the fact that the emergence of the electromagnetic attraction force between quasi-rotating electrons with opposite spins allows overcoming the Coulomb repulsion and promotes stable pairing of the valence electrons of atoms participating in the molecular orbitals.

The spins of electrons can change their spatial direction randomly and very quickly. When, during a collision of atoms due to their thermal motion, the spins of their outer valence electrons accidentally turn out to be antiparallel to each other, then their electromagnetic attraction occurs, resulting in their bonding in molecular orbitals. The proposed electromagnetic mechanism of the formation of paired electrons can explain not only the emergence of molecular orbitals but also the possibility of electron pairing in the orbitals of the atoms themselves.

In the formed molecule, two opposing forces can act. The first is the force of electrostatic repulsion between the positively charged nuclei ( $F_{r,n-n}$ ), and the second is the force of electrostatic attraction between the positively charged nuclei and the negatively charged electrons of the molecular orbital ( $F_{a,n-e}$ ). It is advisable to analyze these forces, which is easiest to do using the example of the hydrogen molecule. It is known that the average distance between nuclei in a

hydrogen molecule is 0.07416 nm, and between nuclei and the molecular electron orbital is 0.03708 nm. This allowed performing calculations using the Coulomb equation, which is valid for atomic and even subatomic levels. The calculations showed that  $F_{r,n-n} = 4.0 \times 10^{-7}$  N, while  $F_{a,n-e} = 26.8 \times 10^{-7}$  N. Thus, the strength of the H-H covalent bond in one hydrogen molecule can be evaluated as  $F(H-H) = 2.28 \times 10^{-6}$  N. As is known the energy of this bond is  $E(H-H) = 4.5$  eV. To break all covalent bonds in 1 mole of hydrogen molecules the force  $F_m(H-H) = 1.37$  EN or energy  $E_m(H-H) = 434$  kJ must be spent.

Thermodynamics provides obtaining data on the energy (E) of other types of covalent bonds, as well. For example, the energy of one covalent bond for oxygen molecule is  $E(O-O) = 2.6$  eV, and chlorine molecule is  $E(Cl-Cl) = 2.5$  eV. For the C-C bond, often encountered in organic chemistry,  $E(C-C) = 3.6$  eV. The covalent bond can be formed also between different atoms. So, the energy of one O-H bond is  $E(O-H) = 4.8$  eV, of one C-H bond is  $E(C-H) = 4.3$  eV, and of one C-O bond is  $E(C-O) = 3.7$ . Generally, the energy of one covalent bond of different types can vary from 2 to 6 eV. The difference in the energy values of one covalent bond is caused by the difference in the bond length, the degree of multiplicity, and the electronegativity of atoms.

Thus, generally, the strength and energy of covalent bonds in molecules depend on the difference between forces of electrostatic attraction between the nuclei and paired electrons of molecular orbitals and the force of electrostatic repulsion between positively charged nuclei, as well as between negatively charged electrons of atomic orbitals of different atoms.

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### 3. Conclusions

A concept of electrons pairing and forming covalent bonds in a molecule was proposed. Analysis of forces acting in the electrons showed that the force of electromagnetic attraction between paired electrons is much greater than the force of electrostatic repulsion. Thus, the valence electrons of neighboring atoms interact with each other like femto-sized electromagnets. It was found that the force of electrostatic attraction between nuclei and paired electrons of a molecular orbital significantly exceeds the force of electrostatic repulsion of nuclei, which ensures the formation of a strong covalent chemical bond. We believe that the formation of a covalent chemical bond occurs because the force of electrostatic attraction between the nuclei and paired electrons of molecular orbitals significantly exceeds the forces of electrostatic repulsion between both the positively charged nuclei and also the negatively charged electrons of the atomic orbitals of different atoms.

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### Compliance with ethical standards

#### *Disclosure of conflict of interest*

The author of this paper declares that there is no conflict of interest.

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