Artificial intelligence, physical substantiation of the chemical bond and synthesis of new substances.

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Abstract: Given the physical justification of the chemical bond as a standing de Broglie wave of valence electrons, it is quite possible to have an accurate theoretical description of the chemical bond (molecules), which will lead to the rejection of the real synthesis of substances. The synthesis of all theoretically possible new substances is practically impossible due to the insufficiency of matter. Therefore, in the future, synthesis will inevitably move to virtual reality, where it will be produced by AI. But, this requires a strict description of the chemical bond.

Keywords: Chemical bond, de Broglie standing wave, synthesis of substances, amount of substances, artificial intelligence, virtual reality.

INTRODUCTION.

Before starting the discussion, let's recall a little history, including L. Pauling's resonance theory.

"…It is important to understand that there are no resonance structures in reality, and the resonance theory is simply a very convenient and intuitive model for describing benzene.

The concept of "resonance" (in L. Pauling's theory of resonance) does not imply a really occurring resonance between the Kekule structures, it is just a good name for the theory. Successful, because it clearly indicates that at the resonance of the Kekule structures a real molecule of benzene is formed, which has an electronic structure intermediate between them (Kekule structures).

And most importantly, I especially note that the real structure of benzene will have energy below the energy of the Kekule structures (that is why the "resonance theory" is a decrease in the energy of the system, and as it is known at real resonance (as a physical process), one can say "ejection" of energy).

...the theory of resonance extended not only to benzene, but also to chemical bonds... in fact it was the only systematic approach to describing the chemical bond. And despite the fact that in a strictly theoretical analysis (within the framework of quantum mechanics) the resonance theory contradicts the principle of quantum superposition, the idea of resonance (that is, the idea of a real physical process) as an approach for studying the chemical bond is very successful and fruitful.

Since it is precisely the idea of resonance that clearly indicates that in the formation of a chemical bond there must be a "zest", that is, a real physical process that leads to the release of energy (bond energy).

The classical, modern representation of the chemical bond, in fact, ignores the physical justification of the chemical bond. From modern ideas, there is no reason why energy should be released when a chemical bond is formed. Conversely, with the concentration of electrons in the inter-nuclear region, that is, when a chemical bond is formed, it is logical to expect an increase in the energy of the system (the Coulomb repulsion between electrons increases)...

L. Pauling spent one year (1926 - 1927) spent in Europe, in the alma of the mother of quantum mechanics. He actually studied quantum mechanics at A. Sommerfeld (Munich) and at the seminars of E. Schrödinger (Zurich), and the great physicists who stood at the origins of quantum mechanics had a profound influence on him.

After this brief (only 1 year) business trip, L. Pauling understood that only quantum mechanics could be the theoretical basis for understanding the chemical bond. Moreover, now it is obvious, the physical essence, the physical substantiation of various processes for it became vital, therefore in the future the theory of resonance was born. Here some explanations are needed.

In the 20-30s of the 20th century, after the birth of quantum mechanics, many great physicists tried to solve the problem of chemical bonding. But all their attempts were unsuccessful, or rather not very successful.

But this should not be taken as a failure, on the contrary, they clearly indicated the problem: if the reason for the formation of a chemical bond is explained by a real physical process (obviously, it should be so), then an acceptable solution could not be found...

The resonance theory is a “pure” chemical theory, the idea of which implies that there must be a physical process (real), which is the reason for the formation of a chemical bond, we assume that therefore Pauling called the theory “resonance theory”. And there is no doubt that only this approach will lead to a full understanding of the chemical bond.

For this, it is necessary to simultaneously apply quantum mechanics and the theory of relativity of A. Einstein... Probably this is the only way... not very simple, but perhaps the only one that will lead to an understanding of both chemical and many physical processes.

How successful is the application of the concept of a real physical process can be demonstrated by the following example. In 1935, in an article by Linus Pauling, L. O. Brockway and J. Y. Beach entitled “The Dependence of interatomic distance on single bond-double bond resonance”... the multiplicity of the bond in benzene was found to be 1.5 (based on two Kekule structures).

But this way of calculating Pauling within the framework of the theory of resonance in 1937 was criticized by William Penney... The essence of the objections is the following: if the multiplicity of the bond in benzene is 1.5, then it follows logically that the heats of formation of benzene and cyclohexatriene (or one of the “resonant” Kekule structures) also coincide, which contradicts the resonance theory (the real benzene

molecule should have a lower energy). From this it follows logically that the multiplicity in benzene should be greater than 1.5 and W. G. Penney received the number 1.62...

As we can see, the concept of a real physical process (since it is a decrease in the energy of a real benzene molecule) led to the understanding that the multiplicity of the bond in benzene should be greater than 1.5, which was shown by quantum chemical calculations (1.67)...

The concept of three-electron coupling explains why there is an increase in the multiplicity: this is a consequence of the interaction of two three-electron bonds on opposite sides of benzene (with different spins), benzene just “shrinks, decreases” a little. Calculations give a multiplicity of 1.66...” [1].

RESULTS AND DISCUSSION.

Five years have passed since the publication of the work from which the quote is given.

I think now there is a good physical basis for what a chemical bond is. This refers to the work “Chemical Bond, De Broglie Waves and Bond Multiplicity” [2].

The history of this work is interesting. In one of the comments on Quora, I clarified that there is no mass defect in the formation of a chemical bond, since an electron is an elementary particle, and therefore, the rest mass of an electron cannot decrease (the issue of a mass defect in the formation of various systems, mainly physical, was discussed, but the chemical system was also mentioned).

I have never seen in the chemical literature that the chemical bond is considered from the position of a mass defect (university textbooks, scientific publications, etc.).

But, I also understood that any bound system implies an inevitable decrease in mass, as the binding energy is released. Therefore, in the formation of a chemical bond, there must still be a mass defect.

But, a chemical bond is not an atomic nucleus, where everything is simple and clear with a mass defect. Nothing worked out for me with the chemical bond and the mass defect... Although I understood and was sure that the chemical bond can and should be described on the basis of the mass defect. Since the mass defect in the formation of any bound systems is a fundamental and inevitable process.

Since my comment, I have thought about this issue periodically. A few years if I'm not mistaken.

And finally, in August of this year, I was able to write an article on the mass defect and chemical bond [3] (Bohr Model of the Atom, Mass Defect and Chemical Bond). It turned out that an electron in a Bohr orbit loses its relativistic mass. Moreover, the loss of mass goes strictly up to the rest mass of the electron - the ionization potential of the hydrogen atom is exactly equal to the defect of the relativistic mass of the electron (on the Bohr orbit).

Further, taking into account the above article, it was possible to give a general physical justification for the chemical bond as a standing de Broglie wave of valence electrons [2] (Chemical Bond, De Broglie Waves and Bond Multiplicity). It was also possible to explain from a physical point of view the multiplicity of the chemical bond - this is literally the linear energy density of the chemical bond, taken in dimensionless units.

It should be noted that a good theory is good because it is true. That is, a correct theory is, as a rule, fundamental and universal. Moreover, it clarifies and expands our knowledge: the chemical bond described on the basis of the mass defect gives an accurate representation of the "velocity" of the electrons in the chemical bond. Moreover, we now know exactly (using the radius of the atom) at what distances any atom will form "strong" chemical bonds, and at what distances – "weak" and "ultra-weak" chemical bonds. And note that all this is calculated elementarily on the basis of experimental data on the atomic radii. Not bad, right?

In the general case, the above description of the chemical bond based on the mass defect should always be correct when any elementary particles form a bound system. That is, if the proton and neutron consist of three different quarks (quarks are elementary), then the proton and neutron must inevitably be described in a similar way. For this, you need to think carefully for several years.... Of course, if you're lucky. And then, we will learn again, something new and interesting, which will deepen and expand our knowledge at a fundamental level.

It must also be pointed out that the above description of the chemical bond should eventually lead to the long-awaited rigorous theoretical calculation of the chemical bond, which should eventually lead us to such an accurate description of the properties of substances on the basis of theory, when the synthesis of new substances will no longer be needed.

This follows from the fact that the de Broglie waves, that is, the "waves of matter" - are real, they really exist in reality. And since the chemical bond is described precisely as a de Broglie standing wave, it means that the correct calculation of the chemical bond (molecule) will inevitably lead us to a complete and correct description of the properties of a particular substance. That is, the synthesis of new substances will no longer be needed at all.

CONCLUSION.

It is worth recalling that the theoretical number of all possible organic compounds is not limited, and therefore their real synthesis is essentially impossible [4]:

"...the amount of all possible organic compounds is theoretically incalculable [2]. That is, for the numbering of all organic compounds, we will not have enough natural numbers... How then can we synthesize them? At least a trillion. At the moment, approximately 100 million organic substances are known. It is quite obvious that it is impossible to synthesize 1 trillion or 100 trillion substances without artificial intelligence, and in

time it will be a very long process (even if it is done by a robot). But, the mass of raw materials for 100 trillion substances requires a huge amount. Moreover, how much these substances will be “interesting” for science is still a question. In this case, you can go through the virtualization of scientific research. What does it mean?

Suppose, in theoretical chemistry, a scientific work will still be written that completely describes the chemical bond (that's what fundamental science is needed for!). Then, in principle, it will be possible to make a complete reliable calculation of the properties of the molecule based on its structural formula. That is, according to the formula, we can fully describe the properties of a particular substance. Note that in this case the calculated properties will not differ in any way from the experimental ones (remember the electronic circuits). That is, for us the question of principle will no longer be: whether a molecule is synthesized or calculated theoretically. A theoretical calculation will already be equivalent to the synthesis of a substance...

Therefore, it is quite logical to entrust this work on “virtual synthesis” to artificial intelligence (the theoretical calculation will be carried out by AI). Moreover, AI can be given the task of calculating what is equivalent to “virtually synthesize”, for example, 100 trillion substances. For the convenience of human use of this knowledge, it would be logical to create a virtual laboratory in which the AI, that is, a virtual synthetic chemist, will synthesize new substances. After such a virtual synthesis, there will be normal work in a virtual laboratory for the purification and identification of substances.

This interface, in fact, chemical virtual reality, will make it possible to create a convenient library of substances. The work of such a virtual chemist (development of synthesis, description, synthesis itself, etc.) will always be online, in the corresponding virtual reality (a real synthetic chemist can always take part in this work)...

It is quite obvious that AI will be the author of scientific papers on the data obtained. Moreover, writing works for him will be the easiest thing. In fact, a virtual chemist becomes an ordinary researcher who will be engaged in science according to a strictly specified algorithm. With the development of AI, the number of substances, synthesis methods, etc., virtual reality itself will increase: first, the number of substances will increase, then laboratories, then the number of virtual research institutes, then megacities, etc. will increase. And at a certain stage we get a typical chemical matrix. In fact, this is inevitable, since the number of substances in organic chemistry is unlimited and people will never be able to synthesize and describe them by hand. Moreover, it will be impossible to do this at any level of human development. Therefore, the transition to chemical virtual reality is inevitable and strictly logical in connection with the development of chemistry.

Note that it is difficult to even imagine the possibilities of chemistry and medicine, when mankind will possess a library of organic substances of 100 or 900 trillion. It is highly probable that among these “virtual substances” there will be effective antiviral substances, which in one or two doses can destroy any virus in

the human body. And this means that then viral epidemics will no longer be terrible for humanity. Let us recall that at the moment in pharmacy no more than 100 thousand individual organic substances are used. Now imagine that our medical library can use 1trillion substances... Can you imagine the level of such medicine? Me not... This example is a clear demonstration of why, over time, virtualization of organic chemistry will inevitably occur, and the synthesis of substances will move to virtual laboratories. Now this sounds rather unusual for us, but it has always been so: everything new is first perceived with some caution...

It is the same with the synthesis of substances in virtual reality: now it seems fantastic, but this is how it will be... This is inevitable...".

Thus, the need to have a rigorous theoretical description of the chemical bond (molecules) is dictated by the very logic of the development of organic chemistry and our society, since in the future, the synthesis of substances will inevitably move into virtual reality, due to the fact that in our reality, matter for the synthesis of all substances, just not enough.

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