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Article 13. Original review of quantum chemistry and 3D modeling of artificial intelligence

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Abstract

This article has reviewed the quantum chemistry theories and case studies in the past, attempting to further improve both theories and methods on quantum chemistry, which provides the new design philosophy of 3D modeling technology.

Key words: Quantum Chemistry Equations, Chemistry Bond, Chemistry Bond Energy, Electron Cloud, Atomic Orbitals, Molecular Orbitals, Electron and Nuclear Wave Functions.

Key features:

1.Introduction: in this paper, the basic theoretical knowledge related to quantum chemistry is fully summarized and reviewed, covering atomic and molecular chemistry bond, the relationship between the strength of chemical bond and structural chemistry stability, the definition of thermo-chemistry and chemical bond energy, three representative methods to compute chemistry bond energy, including molecular orbital (ab initio) algorithm, density functional theory (DFT) algorithm, layered ONIOM (our own n-layered integrated molecular orbital and molecular mechanics), and electron cloud orbital theory. On the basis of full review, this paper combines the application of 3D simulation technology on chemical bond, chemical thermal bond energy and chemical reaction rate, which is designed by my previous article [5], to further discuss the application of three representative calculation methods of chemical bond energy reviewed above on this 3D simulation technology. 译文：本文首先对量子化学相关基础理论知识进行充分总结、回顾，其中主要包括原子与分子化学键、化学键强弱与化学结构稳定性相互关系、热力化学与化学键能定义、三种代表性的计算化学键能主要方法（包括分子轨道从头算法、密度泛函算法、分层的ONIOM）、电子云轨道理论。在充分综述基础上，本文结合本人之前设计的 3D 模拟技术对化学键、化学热力键能和化学反应速率的应用[5]，进一步探讨了以上回顾的三种代表性化学键能计算方法在此 3D 模拟技术中的应用;

2.The conceptions of three types of chemistry bond is modified and redefined,

including ionic bond, covalent bond, metal bond;

3.This article has proposed three new theories underlying the atomic orbitals and correspondingly the new experiment methods are designed to measure the quantum chemistry variables;

4.The thermal dynamics of chemistry bond energy is originally discussed according to the element spectrum experiment;

5.This article has critically discussed the Schrödinger equation and linear combination of atomic orbitals (LCAO). To improve this, my 3D modeling has designed the methods to quantify the relationships of chemistry bond energy to the electron orbital selection, orbital electromagnetic energy and electron electric charges on the basis of experiments;

6.This article has improved the electron cloud theory by 3D modeling;

7.The nuclear wave function is originally discussed according to the NMR experiment, aiming to establish new atom system equations at quantum level.

1.Chemical Bond

1.1.Conception of chemical bond

Chemical bond is a general term defining the strong interaction forces between two or more adjacent atoms (or ions) within a pure molecule or crystal. The forces that bind ions or atoms inside a molecule or crystal lattice (other than between molecules or crystal lattices) are commonly named as chemical bonds, which are generally classified into three types: ionic bonds, covalent bonds and metal bonds[1].

1.2.Ionic bond

It is considered that each of three types (ionic bonds, covalent bonds and metal bonds) possesses different origins. The formation of ionic bonds is simplified as the transfer of electrons between atoms, described by the past theory, which forms positive and negative ions through electrostatic interactions. However, the causes of covalent bonds are relatively complex and controversial. Lewis theory suggests that covalent bonds are formed by the sharing of one or more pairs of electrons between atoms, while other different explanations include valence bond theory, valence layer electron mutual exclusion theory, molecular orbital theory, and hybrid orbital theory. The metal bond is generally considered as the modified covalent bond formed by multiple metal atoms that share free flowing electrons [1]. Another more exact classification method is that chemical bonds are divided into heteropolar bonding and homopolar bonding. The heteropolar bonds, taking NaCl as an example, can be imagined to form by two steps that include the transferring of elections from Na atom to Cl atom, and then resulting in the Coulomb force between positively-charged Na^+ ion and

negatively-charged Cl^- ion. However, it is further to explain that the quantum mechanics theory underlying the 'electron transfer' only aims to the electron energy transfer for the completion of outermost shell in atom [3]. Consequently, this theoretical explanation to ionic bonds formation has already pointed out that the formation of heteropolar bonds is caused by the electron energy transfer between atoms rather than the electron itself transferring between atoms. In my another article [7], the electric current is defined as the energy transfer flow generated by the conduction effect of particles' acceleration motion between two or more electric pulse wave sources, which disagrees with the theory that electric current is caused by the electron movement across atoms in conductor materials (otherwise, there will be a large number of positively charged protons bursting out at high speed, so that all electric conductors are the same as radioactive elements, and this theory is obviously out of date). Consequently, my proposed theory also supports the above theory explaining the formation of heteropolar bonds. In nature, usually when high voltage is imposed by external sources (such as lightning), the free and ionized forms of electron can exist, coupled with radioactive elements.

1.3.Covalent bond

Covalent bond is the stable chemical bond formed in the common space between two or more atoms, where their outer orbit electrons show high probability in occurrence between their nuclei due to the overlap of atomic orbitals, resulting in roughly uniform sharing of electron energy between their nuclei. In the process of covalent bond formation, because the number of unpaired electrons provided by each atom is definite, once an unpaired electron of an atom pairs with unpaired electrons of other atoms, it cannot pair with other electrons again, so that the total number of covalent bonds which each atom can form is definite, which is the saturation of covalent bonds. The saturation of covalent bonds is the key determinant to the quantitative relationship of various atoms binding to each other when the molecule is synthesized, which is one of the intrinsic reasons for the law of definite proportion. The main factor affecting the directionality of covalent bonds is the orbital extension direction. Except for the spherical 's' orbitals, all the other atomic orbitals display as fixed extension direction, so when covalent bonds are formed, the orbital overlap also has a fixed direction resulting in the directionality of the covalent bonds, which further determines the molecular configuration [4]. Another theory explaining the formation of covalent bonds is the homopolar bonds theory. Taking H_2 as an example, the conception of H_2^+ is introduced as molecule-ion, contrasting with the neutral H_2 by removing one electron. Then the remaining electron may jump back and forth between two nuclei, consequently occupying the space between two nuclei. The Coulomb force imposed on the remaining electron may likely balance between two nuclei [3]. However, this theory does not explain where the removed electron leave to. Further more, how can the negative Coulomb energy of only one remaining electron balance the Coulomb energy of two positive nuclei? Obviously, the gas H_2 under normal ambient conditions usually does not show positive charges in the air, so I don't agree with this theoretical explaining by proposing H_2^+ as molecule-ion.

The formation mechanism of covalent bonds is explained by my another article that expands the interactive forces between symmetric spaces as [2]: “For example, there are two covalently bonded atoms (atom1 and atom2). There are electron 1 and proton 1 in atom 1, as well as electron 2 and proton 2 in atom 2, respectively. The negatively charged electron 1 is pulled and paired by the positively charged electron in its correspondingly symmetric three-dimensional space; it is also pulled and paired by positively charged proton 2 in atom 2 due to the covalent bond; the positively charged proton 2 is pulled and paired by the negatively charged electron 2 in atom 2; then the negatively charged electron 2 is pulled and paired by the positively charged electron in its correspondingly symmetric three-dimensional space. This series relationship also exists on electron 2 - proton 1 - electron 1. It's like a series of batteries, from positive to negative, positive to negative... as cyclic connection. This also makes the electron cloud between atoms display as a double - ring crossing mode, so as to form a stable molecular structure. [2]” Here this article further proposed that these two cyclic connections in double - ring crossing mode shows opposite orbital direction against each other due to ‘Pauli exclusion principle’, and the electron energy distribution must be symmetric so that the molecule structure is stable.

1.4.Metal bond

My article defines that the metal is composed of single atom molecule and the metal bonds is caused by the combination of both covalent bond and Van der Waals force between adjacent molecules of single metal atom. The generation mechanism of Van der Waals force is demonstrated in my another article [11].

2.Atomic Orbital

2.1.Conception of atomic orbital

Atomic orbitals, also known as orbital states, interpret the wave motion of electrons in atoms by using mathematical functions. This wave function can be used to calculate the probability of electron appearances in the specific atomic space outside the nucleus of an atom, as to indicate the possible positions of electrons in three-dimensional space. Orbit refers to the region where electrons show a high probability to appear in the outer space of the atomic nucleus, as defined by the wave function. In quantum definition, atomic orbitals are the possible quantum states of individual electrons within electron clouds surrounding the nuclear of an atom, described as orbital wave functions [8].

2.2.The wave function of orbital

The atomic orbital is limited to the wave function of a single atom, which is mainly defined by three quantization parameters: principal quantum number, angular quantum number and magnetic quantum number to determine the energy, angular momentum and orientation of the electron respectively, all of which are collectively characterized by quantum numbers. Each orbit is defined by a different set of

quantum numbers and can accommodate up to two electrons. The ‘s’ orbitals, ‘p’ orbitals, ‘d’ orbitals and ‘f’ orbitals represent orbitals with angular quantum numbers=0, 1, 2 and 3, respectively [8].

2.3.The three fundamental theorems

The motion of electrons along atomic orbitals follows three fundamental theorems: the ‘Principle of minimum energy’, the ‘Pauli exclusion principle’ and the ‘Hunt's rule’. The principle of minimum energy means that when electrons outside the nucleus move, they always prioritize occupying lower energy orbitals, causing the entire system to be under the state of lowest energy; The Pauli exclusion principle is applied to the arrangement of electrons, which can be expressed as: at most two electrons with opposite spinning direction can be accommodated in an orbit; Hund's rule: when electrons are arranged in degenerate orbitals, they occupy different orbitals as much as possible and their spins are parallel. According to the Hund's rule, when the electron layout is completely full, electron configuration is interpreted as s^2, p^6, d^10, f^14; when it is half full, electron configuration is interpreted as s^1, p^3, d^5, f^7; when it is completely empty, electron configuration is defined as: s^0, p^0, d^0, f^0. The above three states are the relatively stable structure [8].

2.4.Principle quantum number

The existence of an electron layer can be proven by the fact of the linear spectrum of hydrogen atoms. Normally, the electrons of a hydrogen atom move along the electron layer closest to the nucleus and do not release energy, which is defined as the ‘ground state’. When a hydrogen atom obtains external energy (such as heat, discharge, radiation energy, etc.), its electrons can transition to the electron layer at longer distance to the nucleus with higher energy, and the state in which the electrons are transitioned into is defined as the ‘excited state’. Inversely, when electrons transition from the electron layer with relatively higher energy to the electron layer with relatively lower energy that is closer to the nucleus, energy is released in the form of electromagnetic waves. Because the electronic layer is discontinuous, the energy released by electronic transitions is also discontinuous correspondingly characterized by the quantized value, and this discontinuous energy is reflected and measured by the spectral line of spectrum. In modern quantum’s mechanical models, the quantum number describing the electron layer is defined as the principle quantum number n, which is given the values of positive integers 1, 2, 3, 4, 5, 6 and 7, corresponding to the electron layer symbols K, L, M, N, O, P, and Q respectively [8].

Table 1. The principle quantum number and its corresponding number of electrons in the 0 family of Chemical periodic table [8].

Principle quantum number	1	2	3	4	5	6	7
Electron layers	K	L	M	N	O	P	Q

Number of electrons in the 0 family	2	2,8	2,8,8	2,8,18,8	2,8,18, 18,8	2,8,18, 32,18,8	

2.5.Electron sub-layer's energy levels

With the increasing of spectral experiments, it has been found that when electrons transition between two adjacent electron layers, multiple similar spectral lines appear. This indicates that there is also slight difference in energy within the same electron layer, which is defined as the 'electron sub-layer' or 'energy level'. The quantum number describing the energy level is defined by the angular quantum number 'l'. In all the chemistry elements from the first to seventh cycles of Chemical periodic table, four energy levels are classified, named as 's, p, d, and f'. The energy levels of s, p, d and f can vary in spectral lines, and this phenomenon is called 'level splitting', which is attributed to the shielding effects caused by the mutual repulsion of electrostatic forces between electrons outside the nucleus, weakening the attraction of electrons at the atomic nucleus. The electrons at the 's' level repel the electrons at the 'p' level, pushing the 'p' electrons away from the nucleus, and there is a similar mechanism between energy levels 'p, d and f' [8].

Table 2. The angular quantum number 'l' at each electron layer [8].

Principle quantum number 'n'	1	2	3	4
Electron layers	K	L	M	N
Angular quantum number 'l'	0	0,1	0,1,2	0,1,2,3
Energy level	1s	2s,2p	3s,3p,3d	4s,4p,4d,4f

2.6.Orientation of electron orbital motion

Under the presence of external magnetic field, many atomic spectral lines undergo finer splitting, which is defined as the 'Zeeman effect' and the splitting caused by external electric field is called the 'Stark effect.' However, this splitting does not exist in the absence of external magnetic or electric field, indicating that although electrons show the same energy at the same energy level, they move in different directions and are therefore subject to Lorentz forces in different directions. The quantum number describing the orbital direction is called the magnetic quantum number symbol 'm'. For each determined energy level (electron sub-layer), 'm' has a fixed value that is independent of the electron layer (principle quantum number), which means that the orbital number of any energy level within the electronic layer is the same [8].

Table 3. The magnetic quantum number at each energy level [8].

Energy level	s	p	d	f
magnetic	1	3	5	7

quantum number 'm'				
Orbital number	1	3	5	7

2.7.Electron spin

Differed from the electron orbital motion orientation around the nucleus, the electron spin defined here is the spinning motion around the center of electron itself, rather than around the nucleus of an atom, which is expressed as spin quantum number 'ms' in addition to the three types of quantum parameters above [10]. Because electrons have 1/2 spin, the energy levels are further divided under external magnetic field [8]. When the electromagnetic wave with a frequency equal to this energy difference is absorbed by electron, it will cause transitions between energy levels and this phenomenon is called electron spin resonance (ESR). The absorption of accompanying electromagnetic waves is called ESR absorption. The conditions for generating ESR are expressed as equation: V_O (MHz) = 1.4·g·Ho (Gaussian). In the equation,V_O is the frequency of the electromagnetic wave, Ho is the strength of the external magnetic field, and g is the Granger factor (g factor). There are many electrons in a molecule, and generally every pair of two electrons have opposite spin, thus canceling out each other, so the net spin quantum number is often 0. In comparison, free radicals have odd number of electrons, with unpaired electrons that have no electron spin to offset. Some molecules, although contain even number of electrons, have two electrons with the same spin direction, resulting in the net spin quantum number of one (such as oxygen molecules). Ions also have net spins, such as constant magnetic ions Cu^{2+}, Fe^{3+}, and Mn^{2+} [9].

2.8.Further discussion of atomic orbital

Firstly, the distribution of electrons' number along each electron layer inside an atom is subject to the three fundamental theorems above. However, my article further proposes that along the radius of an atom from the nucleus to the outermost layer, the distribution of electron numbers tends to display in the form of normal distribution rate. The highest number of electrons is located at the middle of radius of an atom, with the minimum number at the electron layer closest to the nucleus and at the outermost layer respectively. From the middle of radius to both the electron layer closest to the nucleus and the outermost layer, the number of electrons tends to decline. This distribution form reveals that the spatial electron mass distribution is subject to the normal distribution Law along the atomic radius in the outer nucleus spaces of an atom.

Secondly, my another article discusses the anti-particles as: "these magnetic elementary particles' cutting motion along the magnetic line on the fourth dimensional axis is the mechanism of generating electric charges [42], so the spinning motions of elementary particles mentioned above is relative to the magnetic line on the fourth dimensional axis, rather than the rotation motion around the rotation center point of an atom in the three dimensional spaces, but the two kinds of motion orbits

must influence each other.[12]" The electric energy of electrons is discussed as "in the electron clouds, if the free electron with rotation motion of clockwise orientation is emitted from the unstable atom, which is defined as the negative pole relatively to the nuclear of an atom, the nucleus would tend to be positive β decay process; if the free electron with rotation motion of anticlockwise orientation is emitted from the unstable atom, which is defined as the positive pole relatively to the nuclear of an atom, the nucleus would tend to be negative β decay process. Consequently, the electrons can be both positive and negative poles relatively to the nucleus of an atom, rather than single pole to the nucleus. Because the electron's cutting motion along the magnetic line on the fourth dimensional axis is the mechanism of generating negative electric charges in electron clouds, the quantity of electric charges must be different between clockwise spinning electrons and anticlockwise spinning electrons in electron clouds according to the theory about the generating reasons of both positive and negative β decay process: for the positive β decay process, the free electrons of clockwise spinning in electron clouds, which is the negative pole relatively to the nuclear of an atom, carries more negative electric charges; for the negative β decay process, the free electrons of anticlockwise spinning in electron clouds, which is the positive pole relatively to the nuclear of an atom, carries less negative electric charges (Please note: the β particles' mass is considered to be equal to the electrons in electron clouds, but both positive and negative β particles from the decaying nucleus are not the electrons spinning in electron clouds. Do not be confused!). Therefore, it is further to deduce that the free electrons of clockwise spinning are more active in chemistry reaction than the anticlockwise ones. [12]"

My article here further proposes that the electron's orbital sub-layers or energy levels defined by the angular quantum number 'l' above are mainly determined by the clockwise or anti-clockwise rotations around the nucleus of an atom. If the free electrons clockwise rotate at a specific electron layer, which is the negative pole relatively to the nuclear of an atom, carries more negative electric charges/energy, then the electron's orbital sub-layer or energy level is higher; In comparison, if the free electrons anticlockwise rotate at a specific electron layer, which is the positive pole relatively to the nuclear of an atom, carries less negative electric charges/energy, then its corresponding orbital sub-layer or energy level is lower.

Thirdly, as discussed: "these magnetic elementary particles' cutting motion along the magnetic line on the fourth dimensional axis is the mechanism of generating electric charges, so the spinning motions of elementary particles mentioned above is relative to the magnetic line on the fourth dimensional axis [42]," my article here further confirms that the electron spinning motion around the electron itself defined by the spin quantum number 'ms' above is the indicative parameter of electron's cutting motion along the magnetic line on the fourth dimensional axis, which is the mechanism generating the electric charges of electrons. As discussed by my another article "the magnetic moment strength of the electron is 659.59 times higher than the proton in the hydrogen nucleus, and it is easy to understand that the centripetal force

generated by the decomposition of both the coulomb force and magnetic force between positive and negative charged particles in the atom should be opposite in the vector direction with the same force strength, which belongs to the interaction force to achieve mechanical balance. Therefore, the fact that the magnetic dipole moment generated by the electron spin motion is significantly larger than the proton must be explained by the magnetic line in the fourth dimension axis [13].” It is further to confirm that the electron spin motion is definitely the motion characterized by the spin quantum number ‘ms’ above, quantifying the mechanism generating the electric charges of electrons. The Granger factor (g factor) measured by ESR experiment correspondingly becomes this indicative parameter of electron charges. The negative charges carried by each electron vary between different element atoms, so the g factor changes among different element atoms under the same external magnetic field. The electric charges of electron at each energy level of a specific orbital layer that can be reflected by the intensity of each spectral line in spectrum, is the function of the electron spin resonance (ESR), both of which can be exactly measured by experiments independently. The methods in details is discussed below: Step 1. according to the spectral wave length characters, it is to analyze the different electron orbital layers differentiated by different spectral wave lengths; Step 2. according to the intensity at each spectral line of a specific orbital layer, the electric energy of electrons is estimated at each energy level/orbital sub-layer; Step 3. ESR experiment is conducted, it is to estimate the g factor of unpaired electron according to the strength of external magnetic field and the absorbed electromagnetic wave frequency, which is discussed above. The g factor of unpaired electron would indicate the electric charges carried by the electron in an atom; Step 4. The function is established between the intensity of spectrum and the g factor, to quantify the electron cutting motion along the magnetic line on the fourth dimensional axis, generating the electric charges of electrons. Obviously, different element atoms show different ‘g’ factor to reveal that the electric charges of electron vary among different element atoms. If the electrons are all paired in an element atom, then it is to estimate the g factor by its corresponding ionic form.

In section 2.5, the phenomenon of ‘level splitting’ is discussed, which is attributed to the shielding effects caused by the mutual repulsion of electrostatic forces between electrons outside the nucleus, weakening the attraction of electrons at the atomic nucleus [8]. My another article has further proposed that “the neutral shielding effect of the whole atomic structure is the electromagnetic wave principle of the light reflection phenomenon. The stronger the reflection effect of light on the surface of the object, the higher the neutral shielding capacity of the object atoms [43].” In section 2.6, it is discussed that under the presence of external magnetic field, many atomic spectral lines undergo finer splitting, which is defined as the ‘Zeeman effect’ and the splitting caused by external electric field is called the ‘Stark effect’ [8]. Consequently, my article here further proposes that the experimental testing of both ‘Zeeman effect’ and ‘Stark effect’ can reflect the neutral shielding capacity at each electron orbital. The weaker the ‘Stark effect’, the less effect of external magnetic field, and the

stronger neutral shielding capacity at an electron orbital.

After re-definition of these quantum parameters, the electron orbital quantum equations will be modified correspondingly in the next section.

3.Element Spectrum

3.1.Absorption spectrum

Atoms or molecules in the ground state or low excited state absorb light with continuous distribution over certain ranges of wavelengths, transitioning to excited state, which results in the specific spectrum composed of dark lines or bands arranged according to wavelength. The exited process is defined by equation: $\Delta E = E2-E1 = hv = hc/\lambda$, where ΔE is the energy absorption by electrons, E2 is the electron orbital energy of exited state, E1 is the electron energy at lower energy orbital, h is the Planck constant, v is the light wave frequency, c is the light speed and λ is the light wavelength. The background value of the absorption spectrum is the bright continuous spectrum. Through extensive experimental observations, it has been concluded that the position of the dark line in the absorption spectrum of each element coincides with the position of its bright line spectrum of background value, which means that the frequency of light emitted by each element corresponds to the same frequency of light absorbed. Therefore, the dark lines in the absorption spectrum are the characteristic spectral lines of atoms. Studying absorption spectroscopy can reveal the structure and motion of atoms, molecules and many other substances, as well as their interactions with electromagnetic fields or particles [14]. It is to set an example of organic compounds below:

Absorption spectroscopy is commonly used to analyze organic compounds. The UV-visible absorption spectrum of organic compounds is mainly generated by the transition of valence electrons in molecules, which refer to the electrons in an atomic that can interact with other atoms' electrons to form chemical bonds [15]. The valence electrons in molecules are classified into bonded electrons which include ‘s’ electrons and ‘p’ electrons with low energy in orbitals, and un-bonded electrons that include ‘n’ electrons with lower energy in the orbitals. These three types of electrons may absorb certain amount of energy, which transition to higher energy level at anti-bonding orbitals [14]. There are four types of valence electron transition found in organic compounds:

1. s-s* transition. The energy difference of s-s* is large with high energy requirement, and the absorption peak falls in far ultraviolet (l<150nm). For example, saturated hydrocarbons only have s and s * orbitals and can only generate s-s* transitions, such as methane with absorption peaks at 125nm; the ethane absorption peak is at 135nm (<150nm);
2. p-p* transition. The p-p* energy difference is small, so the required energy is low. The absorption peak is in the ultraviolet region (around 1200nm). For example,

unsaturated hydrocarbon molecules have p-electrons and p* orbitals, which can generate p-p * transitions. For example, $CH_2=CH_2$ with an absorption peak of 165nm;
3. n-s* transition. The energy of n-s * is relatively low, with a peak in the ultraviolet region (around 1200nm) that is close to p-p*. It can be generated from organic molecules containing heteroatomic groups such as - OH, - NH2, - X, - S, etc;
4. n-p* transition. The n-p* energy is low, and the absorption peak is in the near ultraviolet and visible regions (1200-700nm) containing unsaturated groups of heteroatoms, such as -C=O, such as acetone that shows both n-p* transition and p-p* transition, with a lmax of about 280nm [14].

Among above four types of valence electron transitions, the order of energy levels required for various transitions is: s-s * > n-s* > p-p* > n-p*. The chemistry substances generating visible colour for spectral analysis of organic compounds are classified into chromophores, which include groups containing p-electrons such as C=C, C=O, COOH, COOR, NO2, N=N and aryl groups, and auxochrome that includes groups containing n electrons such as OH, OR, X, NH2, NO2, SH, etc [14].

3.2.Emission spectrum

In comparison and contrast to the absorption spectrum, the emission spectrum is the spectrum directly generated by object luminescence without background light waves, which is usually thin gas or vapor metals. Emission spectrum is formed by the emission of excess energy when electron at high energy levels transitions to lower energy levels, so the electrons need to be excited before energy emission procedure. Thin gas luminescence is composed of discontinuous bright lines, whose emission spectrum is known as the bright line spectrum. A spectrum containing only some discontinuous bright lines is called a bright line spectrum, in which each bright line corresponds to different wavelengths of light. Usually the bright line spectrum is caused from the emission spectrum of thin gases or metal substances at vapors state. Under this substance state, the bright line spectrum is emitted by atoms in the free state, so it is also called an atomic spectrum. Experiments have shown that different atoms emit different bright line spectra, and each element's atom has an unique bright line spectrum. Each atom can only emit light of specific wavelengths with its own characteristics. Therefore, the spectral lines of the bright line spectrum reveal the characteristic spectral lines of different element atoms. The characteristic spectral lines of atoms can be used to identify substances and study the structure of atoms [16][18]. Compared with the absorption spectrum, each dark line of light spectrum in absorption spectrum correspond to each bright line of emission spectrum, but usually the visible number of dark lines of absorption spectrum is less than the bright lines of emission spectrum [17].

3.3.Hydrogen atomic spectrum

Hydrogen atomic spectrum refers to the spectrum obtained by the emission or absorption of photons at different wavelengths and energy levels by electrons within hydrogen atoms during different energy level transitions. The hydrogen atom

spectrum displays as the discontinuous line spectrum that contains spectral lines ranging from radio waves, microwaves, infrared light, visible light, to ultraviolet light [24].

3.4.Discussion of element spectrum and chemistry bond energy

My another article explains the thermal theory that "the most efficient 'heating' process is the electromagnetic waves from external thermal sources, which have the same frequency as the electromagnetic waves emitted by the molecule motion of receptor objects and show similar amplitude of vibration to the electromagnetic waves emitted by the molecule motion of receptor objects (the amplitude of vibration between these two waves should not show large variation), is able to accelerate the revolution/rotation motion of receptor molecules (or atoms) most effectively. [19]" In my thermal theory, this 'heating' process is attributed to "the effects of stable constructive interference between the external thermal source of electromagnetic waves and the electromagnetic waves emitted from the receptor molecules (or atoms) becomes the major forces of accelerating the electron rotation motion of receptor molecules (or atoms).[19]" Obviously, only two waves of the same wave frequency generate constructive interference. As discussed in 3.1 section above, through extensive experimental observations, it has been concluded that the position of the dark line in the absorption spectrum of each element coincides with the position of its bright line spectrum of background value, which means that the frequency of light emitted by each element corresponds to the same frequency of light absorbed [14]. Consequently, this experimental conclusion further supports my thermal theory proposed in my previous article, which becomes one of the experimental basis to discuss the chemistry bond energy in the next section.

It is to further discuss the formation of dark lines in the absorption spectrum next: in the absorption spectrum, the dark lines display in the background continuously and durably with the working equipment, rather than appearing at transient time. This requires the ground state electrons to transition into excited state, and then the excited electrons immediately transition back into ground state, releasing electromagnetic waves, so that there are always sufficiently free electrons under ground state to absorb the external energy and to form dark lines continuously and durably. In theory, the absorbed electromagnetic energy is equal to the released electromagnetic energy. However, the released electromagnetic energy must be absorbed by the 'black body' effects inside an atom, which is discussed in detail by my next journal article [44], so that the dark lines can occur in the absorption spectrum.

In 3.2 section, the evidence that usually the visible number of dark lines of absorption spectrum is less than the bright lines of emission spectrum may be explained as: there are more orbitals of electrons to be excited in the emission spectrum experiment than the absorption spectrum.

4.Chemistry Valence Formation

4.1.Valence electron

Valence electron is a chemical term referring to an electron in an atom that can interact with other atomic electrons, which forms the chemical bond. The valence electrons of the main-group element are the outermost electrons in the main-group element atoms. For example, the number of valence electrons contained in CO_2 and N_2 are 4+6×2=16 and 5×2=10 respectively. In comparison, the valence electrons of transition elements are not only the outermost electrons, but also contain some of the second outermost electrons and even the third outermost electrons. For example, in lanthanide elements there are also the third outermost 'f' electrons becoming valence electron, which can be determined by atomic orbital energy: ns < (n-2)f < (n-1)d < np. Valence electron orbital arrangement determines the valence electrons, which atoms can use to bond when participating in chemical reactions, and these are the electrons outside the atomic nucleus related to the valence of elements. For example, the valence electron layer structure of chromium is 3d5 4s1, so all six valence electrons can participate in chemistry bonding; Lanthanide elements can also include 4f electrons in the third outer layer. When all the valence electrons participate in bonding, the element valence exhibits the highest normalized valence; When partially participating in bonding, the element valence shows multiple valence characteristics. For example, the highest valence of chromium is+6, in addition to +5,+4,+3,+2,+1, etc [20].

4.2.Main-group element

The main-group element is a kind of chemistry elements referring to the elements in the 's' and 'p' regions of the chemistry periodic table. Another definition of the main-group element is the chemical element in whose atoms the number of electrons in all electronic layers are full of electrons except the outermost one, and the free electron is filled into the 'nS' or 'nP' sub-layer. Element group number is equal to the outermost electron number of the atom (except for rare gases). In the chemistry periodic table, the atomic number of elements in the same main-group gradually increases from top to bottom, the number of electron layers gradually increases, the atomic radius gradually increases, the ability to obtain electrons gradually decreases but the ability to lose electrons gradually increases, so the metallicity of the element gradually increases, while the non-metallic property gradually decreases and the stability of gaseous hydrides gradually decreases. The ions of the main-group elements in aqueous solution (including oxygenic acid radicals) are colorless [21].

4.3.Transition element

Transition elements are the chemical elements in the periodic table that transition from the IIIB group to the VIII group. The common feature of these elements in atomic structure is that the valence electrons are sequentially filled in the d-orbitals of the second outer layer. Sometimes lanthanide and actinide elements are also included in the transition elements. There are three types of elements (scandium to nickel, yttrium transition element to palladium, and lanthanum to platinum), with electrons filling their '3d', '4d', and '5d' orbitals one by one. The characteristic of the

electronic configuration of transition element atoms is that their d-orbitals are not completely filled with electrons (except for Pd), with only 1-2 electrons in the outermost layer. The common Valence electron's orbital arrangement of transition elements includes 3d4s, 4d5s and 5d6s. However, because the energy levels interleave between 4s and 3d, 5s and 4d, 6s and 5d orbitals, and the energy difference between different energy levels is small, in many reactions the 'd' orbital electrons of transition elements can partially or completely participate in bonding [22].

4.4.Molecular orbital method

It studies the motion state of each electron in a molecule from the perspective of the whole molecule, on the basis that the electrons forming chemical bonds move throughout the entire molecule. By solving the Schrödinger equation, the wave function describing the motion state of electrons in molecules can be expressed as Ψ, which is called a molecular orbital. Each molecular orbital Ψ corresponds to each energy level E, which approximately represents the ionization energy of electrons in this orbital. The energy E corresponding to each molecular orbital usually represents the energy level of the molecular orbital, and the total energy of the molecule is the sum of the molecular energy orbital occupied by each electron. It is difficult to solve molecular orbitals Ψ, so approximate solutions are generally resorted to. The most commonly used method is to treat molecular orbitals as linear combinations of atomic orbitals, which is called linear combination of atomic orbitals (LCAO). Molecular orbital theory suggests that chemical bonds are generated by overlapping atomic orbitals, so several atomic orbitals can be linearly combined into the molecular orbitals. According to the theory, when two atomic orbitals overlap, two molecular orbitals can be formed and interpreted as $\Psi = \Psi \pm \Psi$, where the function represents that one of the molecular orbitals is formed by adding the wave functions of two atomic orbitals, called a bonding orbital. In molecular orbitals, the symbols of the wave functions of two atomic orbitals are the same, which means that the wave phase is the same. As a result of the interaction between these two waves, there is a relatively high probability of electron density between the two atomic nuclei. In comparison, the other molecular orbital is formed by subtracting the wave functions of two atomic orbitals, called an anti-bonding orbital, expressed as $\Psi = \Psi - \Psi$. In this molecular orbitals, the symbols of the wave functions of two atomic orbitals are opposite, which means that the wave phases are opposite against each other. As a result of the interaction between these two waves, the wave function values between the two atomic nuclei cancel out. In the region between the atomic nuclei, the probability of electrons appearing is zero, which means that there are no electrons to combine between two atomic nuclei and the two atomic orbitals do not overlap, so they cannot form bonds. The electron cloud density distribution of both bonding and anti-bonding orbitals can also be represented by iso-density lines. On molecular bonding orbitals, the electron cloud density between the two nuclei is high, and its bonding molecular energy is lower than the atomic orbital energy, which facilitates bonding, whereas in the anti-bonding molecular orbit, the electron cloud density between the two nuclei is zero, and its bonding molecular energy is higher than the

atomic orbital energy, making it impossible to form bonds [23].

4.5.Discussion of molecular orbitals

My article firstly disagrees with the LCAO method described above, because obviously the electron orbitals are the discontinuous ones measured by spectrum lines with different wavelength, which means that linear equation is not applicable on the calculation of interaction between two atomic orbitals. Only when two electromagnetic waves possess the same frequency/wavelength, the linear equation is applicable to express the superposition or weakening of both of them. My 3D modeling article simplifies the interaction of chemistry bonds between two molecules into parameter Pa and Pb, which represents the proportion of the specific spherical surface area of active chemistry bonds to its whole spherical surface area of molecule A and molecule B respectively during the molecular revolution, depended on the molecular structure [5]. This modeling methods is also applicable on the atoms within a molecule to model the chemistry bond interaction between two atoms within a molecule. In this modeling method, only once atom A and atom B collides at specific intersection angle (or angles) of spacial magnetism curves between two atom A and B of a molecule, chemistry bonding reaction occurs. The other intersection angles between atom A and B collision can not lead to chemistry reaction. Consequently, my modeling philosophy is still consistent with the LCAO methods modeling electron cloud density described above: “On molecular bonding orbitals, the electron cloud density between the two nuclei is high, and its bonding molecular energy is lower than the atomic orbital energy, which facilitates bonding, whereas in the anti-bonding molecular orbit, the electron cloud density between the two nuclei is zero, and its bonding molecular energy is higher than the atomic orbital energy, making it impossible to form bonds.” However, my modeling philosophy does not agree with that ‘in the anti-bonding molecular orbit, the electron cloud density between the two nuclei is zero.’ In the anti-bonding molecular orbit, the spherical surface area is inactive but the electron cloud density is NOT zero in my 3D model.

In this section, it is to further discuss the electron energy level differentiation on the basis of above review knowledge: in the past theory, the electron energy is not specifically divided into kinetic energy and electromagnetic energy, which needs to be resolved in this quantum chemistry article. My modeling article hypothesizes that the spectrum line wavelengths discussed above indicate the rotation motion’s orbital radius of electron around the nucleus inside an atom. The shorter the wavelength, the shorter radius of electron rotation motion orbitals around the nucleus, the higher frequency of electron spinning motion, so the kinetic energy of electron spinning motion is higher and its corresponding electron orbital layers’ energy is higher as well. However, because only the outermost (or second and third outermost) layers in an atom contain the free electrons that are capable of forming chemistry bonds, the molecular bonding orbitals can be only interacted between the atomic electron orbitals with relatively longer wavelengths measured by spectrum lines. For example, there are six series of spectrum lines found so far in H atom above, so there must be six

electron orbital layers distinguished correspondingly, and only orbital layers with relatively longer wavelength is capable of forming chemistry bonding to interact with other atoms. My modeling article also hypothesizes that the intensity of each spectrum lines indicates the electromagnetic energy of electron in each atomic electron orbital, which is the main energy calculating the active chemistry bonding energy in my quantum chemistry theory. By separating the electromagnetic energy from the kinetic energy at each electron orbital layer, it is to more exactly model the chemistry bonding energy on the basis of experimental methods.

5.Molecular bond shape

5.1.π bond

When the electron orbitals (p orbitals) of two atoms approach from the direction perpendicular to the connecting line between the nuclei of the bonded atom, the electron cloud overlaps and forms the chemistry bond, resulting in the covalent bond called π bond. For example, the connecting line between two bonding atomic nuclei is the xy axis, and the electron 'p' orbital plane of the two atoms is perpendicular to the xy axis, defined as px plane and py plane. If the parts of the orbital plane px and py with the same symmetry are approached or overlapped in a parallel manner along the xy axis, the overlapping part of both px and py is equivalently located on both sides of the xy plane with the same shape but is the opposite phase, showing anti-symmetry towards the xy mirror plane. In this case, the bonds formed by such overlap are called π bonds and the electrons that form π bonds are called π electrons. π bonds typically accompany σ bond formation, and the electron cloud of the π bond is distributed in both top and bottom of σ bond. The electrons of the σ bond are tightly localized between the two atoms forming the bond, while the electrons of the π bond are opposite and can move freely within the molecule distributed between several atoms, so π bonds usually show weaker interaction than σ bond. If the molecule is a conjugated π bond system, π electrons are distributed across the atoms that form the molecule. These π electrons are called delocalized π electrons, and π orbitals are called delocalized orbitals [25].

5.2.σ bonding

The covalent bond formed by the overlapping of two atomic orbitals along the bond axis (the connecting line between two bonding atomic nuclei), is called σ covalent bond which is the covalent bond characterized by an axisymmetric distribution of overlapping electron cloud orbitals along the bond axis in a cylindrical shape. When σ-bonding is formed, the overlapping part of atomic orbitals is cylindrical symmetric around the bond axis, and the shape and symbol of the orbitals remain unchanged when it is rotated at any angle along the bond axis direction. Due to the formation of σ-bonding, the atomic orbitals of the bonding atoms overlap along the bond axis, achieving maximum overlap orbital space, so the σ bond energy is large and the stability is high [26].

5.3. Discussion of covalent bond shape

In section 1.3, covalent bond is discussed as: “these two cyclic connections in double - ring crossing mode show opposite orbital direction against each other due to ‘Pauli exclusion principle’, and the electron energy distribution must be symmetric so that the molecule structure is stable.” This explanation is consistent with the π bond description in 5.1 section, which interprets that “ the overlapping part of both px and py is equivalently located on both sides of the xy plane with the same shape but is the opposite phase, showing anti-symmetry towards the xy mirror plane.”

6.Bond Energy

6.1.Bond energy conception

Bond energy is a kind of physical parameter that measures the strength of chemical bonds based on energy characters. For 1 mol diatomic molecules, the bond energy is the sum energy absorbed by the dissociation of gaseous molecules into gaseous atoms. For 1 mol polyatomic molecules, the energy absorbed by the complete dissociation of a gas molecule into a gas atom with the bond energy is allocated to the energy of each covalent bond in the structural formula, and the sum bond energy of each gas molecule is the standard bond energy unit. Bond energy is usually obtained by measuring dissociation energy through thermochemical methods or spectroscopic experiments, to represent the strength of the specific bond. However, bond energy cannot be used to represent the total amount of energy in substance, but only the free energy difference between the background state and active state. Bond energy also characterizes the strength of chemical bonds and can be measured by the amount of energy required for bond fracture, so it usually refers to the average energy required for each bond when a 1 mol gas molecule is broken down into gas atoms at 101.3KPa and 298K, expressed by Symbol E. For example, the energy absorbed by breaking 1 mol of gas molecule AB into ideal gas atoms at 101.3kPa and 298K is called the dissociation energy of AB (KJ • mol), commonly expressed as the symbol D (A-B). Obviously, for diatomic molecules, the bond energy is equal to the dissociation energy. For example, at 298.15K, the bond energy E (H-H) of H = D (H-H) = 436kJ • mol; However, for polyatomic molecules, bond energy and dissociation energy are different. Taking NH_3 as an example [27]:

NH_3（g）= NH_2（g）+ H（g） D1= 435kJ·mol
NH_2（g）= NH（g）+ H（g） D2= 397kJ·mol
NH（g）= N（g）+ H（g） D3= 339kJ·mol

Formula of bond energy for calculating enthalpy change is expressed as: ΔH = total bond energy of reactant - total bond energy of product. The relationship between bond energy and total substance energy is interpreted as: the higher the bond energy, the lower the total substance energy. The lower the bond energy, the higher the total substance energy. As reactants, substances need to absorb heat during the reaction process to reach the critical bond energy (such as combustion point). The lower total

substance energy of reactants leads to more stable structure and higher bond energy, which absorbs more heat to reach the critical bond energy, whereas higher total substance energy results in unstable structure and lower bond energy, so lower heat absorption is required. Consequently, bond energy refers to the energy released during the formation of chemical bonds or absorbed during the breaking of chemical bonds, which can be used to indicate the strength of chemical bonds and stability of molecule structure [27].

6.2.Discussion of chemistry bond energy

By reviewing this section knowledge, it is to further deduce that the intensity of spectrum lines at relatively longer wavelength indicates the total electromagnetic energy of electrons at relatively outermost orbital layers, which is inversely proportional to the chemistry bond energy activating the chemistry reaction, so the higher intensity of spectrum lines reflects lower chemistry bond energy required for electrons to transit between background state and excited state, and the molecular orbital structure is more unstable correspondingly. Further more, according to the discussion in section 3.4. of this article, the most efficient way of heating process for an atom to reach chemistry bond energy is to absorb the external electromagnetic waves at the same frequencies corresponding to the electron rotation at relatively outermost orbital layers, so that the free electrons at the outermost orbital layers can be activated or excited efficiently, which becomes the most efficient thermal dynamics based on chemistry bond energy.

My 3D modeling paper [5] has designed the chemistry bond energy as parameter Ea and Eb, on the basis of philosophy that ‘constant j and k are given to the clockwise spinning electrons and anticlockwise spinning electrons in electron clouds respectively, when the quantity of electric charges is modeled to represent the difference in electric charges between the two types. For the electrons with higher electric charges, the total electron energy is higher, the chemistry bond energy required to activate the reaction is lower, so the chemistry reaction is more active correspondingly. ’ Consequently, the electron charges’ parameter that is reflected by the g factor of ESR experiment as discussed in section 2.8 above would be used to establish the function between g factor and intensity of spectrum lines at relatively outermost orbital layers, which quantifies the relationship between the total electron energy and chemistry bond energy in my 3D modeling.

7.Bond Length

Bond length refers to the average distance between the nuclei of two atoms A and B forming covalent bonds, which can be measured experimentally. For the chemical bonds composed of the two atoms A and B, if the bond length value is smaller, the bond strength is stronger; if the amount of the bonds is more massive, the bond length is smaller [28].

In atomic crystals, the smaller atomic radius results in the shorter bond length and the greater bond energy. The atomic radius of bonded atoms can be derived from a large number of bond length values; Inversely, the typical bond length of this chemical bond can be obtained by using the sum of atomic radii [28].

For the comparison of covalent bond lengths, the following methods can be generally summarized into: the stronger the covalent bond strength, the smaller the bond length; the greater the difference in electronegativity between atoms to form a covalent bond, the smaller the bond length; However, the bond length is also affected by the type and strength of other chemical bonds formed by that atom [28].

Actually, there are many factors that affect bond length and bond energy, such as atomic radius, distance between atomic nuclei, repulsive force between lone pair electrons, feedback bonds, etc. In actual molecules, due to the influence of conjugation effects, spatial hindrance effects, and adjacent group electronegativity, even the same chemical bond length still varies under different effects [28].

The numerical values of bond lengths in various molecules have been commonly determined by the experiment of X-ray diffraction of crystals; a few of simple gaseous molecules and X-H bond lengths have been measured by spectroscopy and neutron diffraction methods [28].

Table 4. Examples of bond energy and bond lengths [28].

Chemical Bond	Bond length/(10^-12m)	Bond energy/(kJ/mol)
Br—Br	229	193
C—B	156	393
C—Br	194	276
C—C	154	332
C═C	134	611
C≡C	120	837
H—Br	142	366
H—Cl	127	431
H—F	92	565
H—I	161	298
H—H	75	436

Through comparison, it can be found that the bond lengths of chemical bonds H-F, H-Cl, H-Br and H-I increase sequentially with the increase of atomic radius, while the bond energy decreases sequentially; The bond lengths of single, double and triple bonds of C-C, C═C and C≡C decrease in sequence, but the bond energy gradually increases. However, the bond lengths of double and triple bonds are not two or three times that of single bonds [28].

8.Electron Cloud

8.1. Electron cloud conception

Electronic cloud is a kind of modern statistical method used to depict the distribution of electrons in extra-nuclear space, differed from the planetary orbital model. Electrons possess the property of wave particle duality, without a fixed and defined orbit like the motion of macroscopic objects, so their trajectory can be hardly drawn. It is seemingly impossible to predict where the electron appears in the outer space at a transient moment, but it is feasible to know the chances of its appearance at the specific location. Therefore, the probability of electron occurrence per unit volume space, i.e. the probability density, is expressed as the density of small white dots. A dense area with small white dots indicates a high probability density of the appearance of electrons, while a sparse area with small white dots indicates a low probability density. This model looks like a negatively charged cloud surrounding the atomic nucleus, hence it is called an electron cloud, which differs from the planetary orbital model that attempts to simulate the real motion orbitals in atom [29].

In quantum chemistry, it is to use a wave function Ψ (x, y, z) to characterize the motion state of electrons with its mode $|\Psi|^2$. This value represents the probability density of electrons appearing somewhere outside the nucleus per unit volume space, so the electron cloud is actually the distribution of $|\Psi|^2$ value in space. The study of the spatial distribution of electron clouds mainly includes two parameters: radial distribution and angular distribution. The radial distribution explores the relationship between the probability of electron occurrence and the distance from the nucleus, and is regarded as the probability of electron occurrence in a thin spherical shell with a radius of parameter r and a thickness of parameter dr. The angle distribution discovers the relationship between the probability of electron appearance and the angle. For example, s-state electrons have a spherical symmetric angular distribution, and the probability density of electrons appearing in different angular directions on the same sphere is the same. The p-state electrons appear in an 8-shaped form, with varying probability densities in different angles and directions [29].

$|\psi|^2$ represents the probability density of electrons appearing at the specific space outside the nucleus, so the product of the probability density and the total volume of the spaces is the probability of electron occurrence. Each electron outside the nucleus has its own state of motion, represented by each wave function ψ1S, ψ2S, ... and its corresponding probability density $|\psi 1S|^2$, $|\psi 2S|^2$,....; These wave functions and probability densities are different among electrons, so electrons in different states have their own electron cloud distributions [29].

Electronic clouds form different shapes, represented by the symbol s, p, d, f, g, and h. The S electron cloud is spherical and symmetrical, with the same probability of electrons appearing in any direction at the same radius outside the nucleus; The p-electron cloud appears when the principal quantum number n≥2. The 2p electron

cloud is in the shape of a dumbbell and displays in three orientations, namely 2px, 2py, and 2pz. For example, the probability density of p-electron clouds with n=2 and l=1 is the highest appearing in one direction, while the probability density of occurrence in the other two directions is zero; The d electron cloud appears when n≥3; The f electron cloud appears when n≥4 [29].

Iso-density plot is commonly applied to characterize electron density distribution. The points with the same $|\psi|^2$ are connected together to form an iso-density map. For hydrogen atoms, equi-density surfaces are many concentric spheres, and the numerical values in the figure represent the relative magnitude of probability density [29].

At the same energy level, each electron cloud shows the same energy. At the longest distance from the atomic nucleus, the probability density is zero in the atom, which means that it is very unlikely to find electrons there. In areas very close to the nucleus, the probability of electrons appearing is also zero, indicating that electrons cannot reach this region [29].

8.2.Discussion of electron cloud modeling

My 3D modeling paper [5] improves the 3D electron cloud by introducing the electron rotation orientation parameter into sub-model, based on the hypothesis that in the same spacial grid of an atom divided by the sub-model, the electron rotation orientation is simplified into the same directional ones (either clockwise or anticlockwise) in a spacial grid, because only the same directional electrons can conduct rotation motion parallelly and adjacently in a spacial grid of an atom (otherwise they easily repel each other to leave this spacial grid). Consequently, this is an improvement to 3D modeling of electron cloud. Additionally, the wave function of Ψ (x, y, z) can be incorporated into my 3D modeling to calculate the electron density as well.

9.Quantum Chemistry Equations

There are three families of representative equation systems introduced and discussed in this section [6].

9.1.Ab initio method

9.1.1. Introduction of method

In quantum chemistry calculations, ab initio method refers to a kind of quantum chemical calculation method that directly solves the Schrödinger equation based on the fundamental principles of quantum mechanics. The characteristic of ab initio calculation method is that it contains no empirical parameters and does not make many simplifications into the system, whose various chemical systems are calculated by using essentially the same method [30].

To improve ab initio method, the Born Oppenheimer approximation (BO approximation, also known as adiabatic approximation) is a commonly used approximation method for solving quantum mechanical equations of systems containing both electrons and nuclei. When dealing with molecules or other systems using quantum mechanics, it is necessary to obtain the system wave function by solving the Schrödinger equation or other similar partial differential equations, which are often very difficult or even impossible due to excessive system freedom. However, according to the Born Oppenheimer approximation, it is to consider that the mass of an atomic nucleus is much larger than that of an electron, typically 3-4 orders of magnitude larger, so the electrons move much faster than the nucleus under the same interaction. Based on this difference in speed, the electron is simplified into the state moving in the potential field composed of a stationary atomic nucleus at every moment, while the nucleus cannot sense the specific position of the electron so it can only receive the average force imposed by all the electrons. After this simplifying hypothesis, it is possible to achieve the separation of approximate variables between atomic nucleus coordinates and electronic coordinates, and the complex process of the wave function of the entire system is decomposed into two relatively simple processes: solving the electronic wave function and solving the atomic nucleus wave function [30].

Under the Born Oppenheimer approximation, the system wave function can be written as the product of the electron wave function and the nuclear wave function [30]:

$$\Psi_{total} = \Psi_{electronic} \times \Psi_{nuclear}$$

My 3D modeling adopts this system wave function, and consequently the conception of nuclear magnetic resonance (NMR) is reviewed below in addition to the electron wave function.

9.1.2.Nuclear magnetic resonance and nuclear wave function

Atomic nuclei are the positively charged particles, nuclei that cannot spin do not show magnetic moment, while nuclei that conduct spin motion result in circulating current, generating magnetic field to form magnetic moment (μ)[31].

$$\mu = \gamma P$$

In the equation, P is the angular momentum moment, and γ is the magnetic spin ratio which is the ratio between the magnetic moment and angular momentum moment of the spin nucleus, and therefore becomes the characteristic constant of various nuclei [31].

When the spin nucleus is under the external magnetic field with magnetic induction intensity of B0, it will also move around B0 in addition to its spin motion, which is very similar to the motion of a gyroscope called a Lamar process. Angular velocity of spin nucleus precession (ω0) is directly proportional to the induction intensity of the

external magnetic field B0, and the proportional constant is the magnetic spin ratio γ [31].

$$\omega 0 = 2\pi \times \nu 0 = \gamma \times B0$$

In the equation ν0 is the precession frequency.

To transition from a low energy state to a high energy state, the spin nucleus must absorb the energy ΔE by receiving a certain frequency of electromagnetic wave radiation under the external magnetic field. When the radiation energy is exactly equal to the energy difference between the two different orientations of the spin nucleus, the spin nucleus in the low energy state absorbs electromagnetic radiation energy and transitions to the high energy state, resulting in the phenomenon called nuclear magnetic resonance (NMR). When the emission radiation frequency is ν, and the radio frequency is irradiated on the spin system, the energy of this radio frequency is absorbed by nuclei. Therefore, the conditions required for nuclear magnetic resonance are expressed as equation [31]:

$$h\nu = \Delta E$$
$$\Delta E = \gamma \times h \times B0/2\pi$$
$$2\pi\nu = \gamma \times B0$$

9.1.3.Discussion of nuclear wave function

As defined in 9.1.2 section by nuclear conception that “Atomic nuclei are the positively charged particles, nuclei that cannot spin do not show magnetic moment, while nuclei that conduct spin motion result in circulating current, generating magnetic field to form magnetic moment.” Consequently, my article further deduces that the elementary particles, which conduct spin motion cutting along the fourth dimensional axis magnetic lines, become the protons that carry positive charges, while the elementary particles, which cannot spin and do not show magnetic moment, become the neutrons that can not carry electric charges. However, this definition has been further improved by my next article of this journal [44].

My 3D modeling hypothesizes that the emission radiation frequency ν in an NMR experiment indicates the nuclear proton rotation motion frequency, because the frequency of radiation wave emitted by nuclei rotation motion must correspond to the same frequency of radiation wave energy absorbed by the nuclei. It is to further hypothesize that the magnetic spin ratio γ indicates the positive charges carried by protons, because γ becomes the characteristic constant of the specific nucleus and varies among different nuclei, which is caused by the theory that the positive charges carried by each proton vary among various element nuclei. Consequently, the nuclear wave function can be deduced, based on the variables of both ν and γ. Finally, the system wave function can be written as the product of the electron wave function and the nuclear wave function.

9.2.Density functional theory

Density functional theory (DFT) is the quantum mechanical method for studying the electronic structure of multi electron systems. Density functional theory has extensive applications on both physics and chemistry, especially in studying the properties of molecules and condensed matter, which becomes one of the most commonly used methods in the fields of condensed matter physics and computational chemistry. The classic methods of electronic structure theory, especially the Hartree Fock method and its derived method, are based on complex multi electron wave functions, which is difficult to be implemented. To improve this, the main objective of density functional theory is to replace the wave function by electron density theory as the fundamental quantity for research. The multi electron wave function contains 3N variables (N is the number of electrons with each containing three spatial variables), but electron density is only a function of three variables, so that it becomes more convenient to handle both conceptually and practically [32].

DFT is based on two theoretical hypotheses: Hohenberg Kohn's first theorem states that the ground state energy of a system is only a functional of electron density, and Hohenberg Kohn's second theorem proves that the ground state energy is obtained by minimizing the system energy with the ground state density as a variable [32].

9.3.ONIOM computing package

ONIOM is the Gaussian-based computing software applied in quantum chemistry. Gaussian is a powerful quantum chemistry comprehensive software package, whose executable program can run on different models of large computers, supercomputers, workstations, and personal computers, and there are corresponding versions. Gaussian functions include transition state energy and structure, bond and reaction energy, molecular orbitals, atomic charges and potentials, vibrational frequencies, infrared and Raman spectra, nuclear magnetic properties, polarizability and hyperpolarizability, thermodynamic properties, reaction pathways, and its calculations can be performed on the ground or excited states of the system. It can predict the energy, structure, and molecular orbitals of periodic systems, which can therefore serve as a powerful tool for studying many topics in the field of chemistry, such as the effects of substituents, chemical reaction mechanisms, potential energy surfaces, and excitation energies [33].

Studying the reactions and spectra of large molecules, Gaussian 03 has made significant modifications to ONIOM, enabling it to handle larger molecules (such as enzymes), and to study the reaction mechanisms of organic systems, cluster models of surface and surface reactions, photochemical processes of organic compounds, substitution effects and reactions of organic and organometallic complexes, and homogeneous catalysis. Other new features of ONIOM include customizing molecular mechanics force fields; Efficient ONIOM frequency calculation; Calculation of electrical and magnetic properties by ONIOM [33].

10.Case Studies

This section has selected the recent research corresponding to the above representative equation systems for review study.

10.1.NO is one of the main chemical reaction products in the high-temperature air flow field of hypersonic aircraft, and the radiation generated by its vibrational transition is in the typical band of infrared detectors. This research calculates the molecular potential and permanent dipole moment of NO molecule after splitting by using ab initio calculations, and the linear strength of NO molecule at the temperature of 8000 K has been estimated; At temperatures of 300 K and 3000 K, the current theoretical calculation results show good agreement with the data in the HITRAN database; This research has also used a narrowband model to calculate the absorption coefficient of the X2Π1/2 state for NO molecule at temperatures of 296 K and 2000 K. The current method can obtain more line positions for both low and high vibration dynamics than the HITRAN database without relying on experimental spectral constants, efficiently providing high-temperature spectral data of NO molecules for the calculation of target radiation characteristics in numerical wind tunnels [34].

10.2.In this study, ab initio molecular dynamics method has been used to simulate the reaction path of two objects' collision. This method neither assumes any reaction mechanism in advance nor constructs a potential energy surface, but provides random initial conditions for the reactants, including random initial coordinates, random initial velocities, and random initial orientations. Firstly, it is to fix the initial random atomic nucleus position, and then calculate the Schrödinger equation of the electron to obtain the potential energy of the system. Based on the first derivative of potential energy, it is to obtain the force variable. The atomic nucleus moves under the action of this force field, reaches a new position, and then cycles until the reaction ends. By modifying the module of quantum molecular dynamics in the quantization software NWChem, molecular dynamics path calculations of ab initio is performed at the theoretical level of DFT/M06-2x/aug-cc-p VDZ (LANL2DZ-ECP). Through the study of the reaction pathway of the target system, a total of 7 reaction types have been discovered in this article, including 6 bimolecular nucleophilic substitution reaction mechanisms [35].

10.3. Based on the density functional theory calculations, the adsorption and CO_2 catalyzed hydrogenation reactions, which is synthesized by H_2 and CO_2 on nitrogen-doped-graphene-supported-single-atom Zr catalyst (Zr Nx-Gr), have been studied. The adsorption energies of both H_2 and CO_2 on Zr N3-Gr alone are -0.49 eV and -2.17 eV, respectively. In the CO adsorption state of H_2 and CO_2, the adsorption energy is -2.24 eV, which is higher than the adsorption energy on the Zr N4-Gr surface, indicating that the Zr N3-Gr surface is more conducive to the occurrence of CO_2 hydrogenation reaction. On the Zr N3-Gr surface, CO_2 maintains its unique

adsorption characteristics after CO adsorption, weakening the adsorption of H_2 molecules. The catalytic hydrogenation reaction of CO_2 on the surface of Zr Nx Gr starts with the CO adsorption configuration of H_2 and CO_2, forming formate (HCOO *) intermediates along the trans HCOOH pathway. Then, the HCOO * group adsorbs H atoms to form trans formic acid. The reaction energy threshold of this pathway on the surfaces of Zr N3-Gr and Zr N4-Gr are 1.85 eV and 2.48 eV, respectively. The other pathway is the reaction between CO and H_2O, and the reaction energy threshold on the surfaces of Zr N3-Gr and Zr N4-Gr are 1.86 eV and 1.73 eV, respectively, This indicates that Zr N3 Gr is more conducive to the hydrogenation of CO_2 for formic acid, while Zr N4 Gr surface is more conducive to the production of CO [36].

10.4. Graphite phase carbon nitride loaded metal can be used to prepare single atom catalysts with high catalytic performance. This work uses the relativistic and full electron density's functional theory to study the coordination of g-C_3N_4 (CN) structural units and the behavior of stable metals. It is to explore the structure, ligand metal interaction, and single electron reduction properties of the formation of complex [M (CN)] z+(M=Sc, Y, La, Ac, and U; z=2 and 3). Calculations have found that the ligand coordinates with the central ion through six M-N coordination bonds, with each bond strength ranging from -0.79 eV to -0.47 eV. For Sc complexes, single electron reduction mainly occurs at the metal center, while La and U complexes are the ligand reduction mechanisms of metal modification. The ligand and metal of the Y complex are uniformly reduced, while the reducing electrons of Ac complexes are completely captured by ligands by contrast, with almost no involvement of metals. Electronic structure studies have shown that [U (CN)]3+ has three U (5f) single electron of high occupancy orbitals, indicating that the central U is in the trivalent oxidation state. Although [U (CN)] 2+ has four U (5f) single electron orbitals, the contribution of the ligand cannot be ignored, which means that the oxidation state of its U center is between divalent and trivalent [37].

10.5.The reaction mechanism of VAPO-5 molecular-sieve catalytic-oxidation of benzene to phenol has been studied by using ONIOM method. Firstly, aluminum phosphate molecular sieves are synthesized by using pseudo thin water aluminum, phosphoric acid, and ammonium metavanadate as the reactant ingredient sources of aluminum, phosphorus, and vanadium respectively in a fluorinated system based on both single and composite templates. The effects of dynamic crystallization conditions on the crystallinity and morphology of D-VAPO-5 molecular sieves have been investigated, which play the key role in catalyzing the oxidation of benzene to phenol reaction. The experimental results show that the catalytic performance of D-VAPO-5 zeolite synthesized with composite template (TEA and CTAB) is better than that of W-VAPO-5 zeolite synthesized with single template (TEA) in benzene oxidation. Compared with the static method, the D-VAPO-5 molecular sieve synthesized by the dynamic method has higher crystallinity and better catalytic performance. Subsequently, multi-stage porous-aluminum phosphate molecular-sieves have been synthesized by using dynamic hydrothermal method based on different organic

amines as templates. The effect of templates on the configuration of the synthesized molecular sieves has been investigated, and the catalytic performance of D-VAPO molecular sieves with different configurations is evaluated according to toluene oxidation reaction as a probe reaction. The effects of reaction conditions and material quality on toluene oxidation reaction are also investigated [38].

Finally, the ONIOM method is used to study the reaction mechanism of VAPO-5 molecular sieve catalytic oxidation of benzene to phenol. The transition states, intermediates, and reaction energy barriers during the reaction process are analyzed, and the effect of solvent acetonitrile on the VAPO-5 molecular sieve catalytic oxidation of benzene to phenol reaction is calculated accordingly. The calculation results show that in absence of catalyst action, one O atom in H_2O_2 forms a ternary ring with two Cs on the benzene ring, followed by the formation of phenol. The process of forming phenol is a decisive step, with an energy threshold of 296.8 kJ/mol. Under the action of catalyst, the benzene oxidation reaction is divided into four steps: the first step is to form a V-OOH structure between H_2O_2 and V on VAPO-5 molecular sieve; In the second step, OH in V-OOH reacts with H on the proton acid site in VAPO-5 molecular sieve to form H_2O; The third step is to form phenol, and the fourth step is the desorption of phenol molecules from the molecular sieve. The third step is the speed determination step, with an energy threshold of 204.8 kJ/mol. In the presence of solvent acetonitrile, the changes in energy threshold from the first to the fourth step are -2.0 kJ/mol, +1.9 kJ/mol, -30.0 kJ/mol, and -23.7 kJ/mol respectively. The third step is also the rate determination step, with a reaction energy threshold of 174.8 kJ/mol. It is concluded that the addition of solvent acetonitrile reduces the required activation energy threshold for the reaction [38].

Table 5. Summary of case studies.

Case study	Equation System	Study Objectives
[34]	ab initio; HITRAN database	the molecular potential and permanent dipole moment of NO molecule; absorption coefficient
[35]	ab initio; Schrödinger	molecular dynamics path; 7 reaction types; 6 bimolecular nucleophilic substitution reaction mechanisms
[36]	Density Functional Theory	the adsorption and CO_2 catalyzed hydrogenation reactions; Zr Nx-Gr catalysis pathways.
[37]	Density Functional Theory	the coordination of g-C_3N_4 (CN) structural units and the behavior of stable metals; the structure, ligand metal interaction, and single electron reduction properties of the formation of complex [M (CN)].
[38]	ONIOM	the reaction mechanism of VAPO-5

		molecular sieve catalytic oxidation of benzene to phenol; The transition states, intermediates, and reaction energy barriers during the reaction process.

11.Conclusion

By reviewing the past case studies in quantum chemistry, the better understanding of the modeled chemistry theories, the re-occurring of modeling results under changing reaction conditions, and the application of quantum chemistry modeling on engineering would be the main considerations to further develop this model, especially when the computing capacity has been largely enlarged to date. The key features of this study have been outlined at the beginning of this article, and the 3D modeling will be edited according to the improved theories and methods of quantum chemistry substantially discussed in each section of this study. It is expected to develop this 3D modeling project by team work in the mode of open source coding.

Here it is further to conclude the electromagnetic wave theory: for the visible light waves, the electrons' rotation around the nucleus inside an atom becomes the source generating visible light waves, so this electron rotation orbital's angular velocity determines the light waves' frequency and this rotation motion model indicates that light waves are the transverse waves, differed from the longitudinal wave generated by the rays' motion model that is discussed in my another article [39], which further deduces that the six series of spectrum lines found in H atom would correspondingly indicate different colour wavelengths of light waves.

This article has re-defined the ionic bonds as 'electron's energy transferring among adjacent atoms', rather than electron itself transferring, because usually under the ambient normal conditions, atom can be hardly turned to the free state of ions. Only when high intensity of ionization voltage is imposed externally, free state ions will maintain its balance status between internal and external Coulombic force, so it can keep its ionization state. Consequently, it is further concluded that the lightning occurrence that yields high voltage is one of the preconditions generating free state ions or charged particles, which are used to explain and predict the generation of tornadoes and earthquake process in my articles [40][41].

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