

Research Article

The principle and application of experimental method for measuring the interaction energy between electrons in atom

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Received: 22 February 2016

Accepted: 12 March 2016

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ABSTRACT

In the calculation of the energy of atoms and molecules, it is very difficult to calculate the interaction energy (especially the electron pairing energy). A way to solve this problem has been found- The experimental principle of measuring the electron pairing energy is found, a simple and practical method to calculate the interaction energy and atomic energy is invented. The process of getting this kind of method is introduced. At last, the energy of carbon, nitrogen, oxygen and other atoms are calculated by this method. By using this method, the energy of the atom can be calculated by atomic number, and the accuracy can reach more than 95%. Although the technology content of this method is not high, but its practical value is high. The research results presented in this paper have three highlights: (a) The relationship between “the interaction energy of electron-electron, atomic energy” and the nuclear charge number have been summed up; (b) the experimental principle of measuring the interaction energy of electrons is established; (c) the fitting calculation method of quantum mechanics is invented. These highlights have enlarged human knowledge. I solved the problem of computing the interaction energy between electrons in atoms. A simple and effective method for calculating atomic energy is summarized. These techniques are important findings in scientific research, not only increase the knowledge of human beings, but also have broad application prospects. Past times, calculation of the interaction energy between electrons in atoms is a headache. Now the trouble is finally eliminated. The phenomenon-law of the relationship between electron pairing energy and ionization energy has a strong practical. This phenomenon-law reflects the electronic interaction and the mechanism of the electronic structure is the cradle of gestation of new theory. Please note: There is neither lowliness nor nobleness in the law of nature; As long as there is a new discovery, that is, there are the contributions to mankind (have increased human knowledge). The value of the research results is the key to its application prospects.

Keywords: Nuclear charge number, Ionization energy, Electron pairing energy, Interaction between electrons, Perturbation method

INTRODUCTION

The methods used in the calculation of the atomic and molecular calculations include the variational method, the perturbation method, and the *ab initio* calculation. Among these methods, the most troublesome is the calculation of the interaction energy between electrons (in

particular the electron pairing energy). Because there is no real way to overcome this kind of computational difficulty, people use the method of the combination of subjective and objective. That is to say, the subjective factors still play an important role in the existing methods of quantum mechanics. For example, these methods are not subject to the subjective establishment of the model is

to use the trial function. Whether it is the use of subjective model or the use of trial functions are the makeshift process of the subjective logic, rather than rigorous process. For the calculation of the same helium atom, different people use different trial functions; the same person cannot explain why you can use such a trial function. Temptation is a kind of assumption. If it is correct to see whether the final result is consistent with the facts. Since the model is subjective, even if the calculation results are consistent with experimental results, it is only out of work. This is the present situation of quantum mechanics calculation of complex systems.

By using the method of regression analysis, the formula for calculating the interaction energy between electrons and the atomic energy is obtained. The accuracy of the calculation result is also very good. It solve the problem that the interaction energy between electrons in atoms and molecules can be difficult to calculate accurately in the original exist. Applying these regression equations, the energy of all atoms can be calculated only according to the atomic number. The accuracy of the results can meet the general requirements. Although the method is simple, it has high application value. Although the method is simple, it has high application value. It can relieve the suffering of the atomic energy calculation of thousands of people.

In this paper, the energy unit is KJ/mol. Just in some illustrations, the unit on Y-axle is MK/mol, because the energy is too large.

METHODS

Principle of measurement of the interaction energy between the electrons in atom

Can we directly measure the interaction energy between the electrons in atoms by means of the experimental method? No one has done this before. This paper will provide the principle of this experimental method. Whether the experimental method can be used to measure the interaction energy between electrons in an atom environment? Others can not I can.

There are some regularities hiding in the data of interaction energy. As long as careful thinking, these rules can be summed up.

In helium atom, what is the difference between the ionization energy of the two 1s electrons? The ionization of the first electron requires interaction with another electron and the nucleus at the same time (the corresponding energy to be marked as $I_1 = E_{e-n} + E_{e-e}$. Here, E_{e-n} is the interaction energy between electron and nucleus, and E_{e-e} is the interaction energy between electrons), but the ionization of the second electron only requires interaction with the nucleus (the corresponding energy to be marked as $I_2 = E_{e-n}$). This means that the difference in ionizing energy is the interaction energy

between the two paired electrons ($I_1 - I_2 = (E_{e-n} + E_{e-e}) - E_{e-n} = E_{e-e}$) (metering it with dissociation energy). So, we have obtained the calculation formula of the interaction energy of paired electron $1s^2$:

$$E_{e-e}(1s^2) = \Delta I(1s^2) = I_{\text{lastsecond}} - I_{\text{lastfirst}} \quad (1)$$

This is also the working principle for using experimental method to measure the interaction energy between $1s^2$ electrons. This is also the working principle using an experimental method to measure the interaction energy between $1s^2$ electrons. Previously, others do not know that the ionization difference is the interaction energy between electrons in atom. If metering it with system energy, it must be positive value. The general formula for the application of the $2s^2$ for each element is

$$E_{e-e}(2s^2) = \Delta I(2s^2) = I_{\text{last3rd}} - I_{\text{last4th}} = I_{Z-Z-3} - I_{Z-Z-4} \quad (2)$$

For the ns^2 paired electrons, we have $E_{e-e}(ns^2) = (I_{Z-Z-1} - I_{Z-Z-2})/n^2$. Where, Z is the nuclear charge number, n is the principal quantum number is also energy series. If metering with ionization energy, E_{e-e} is negative; it indicates that the system release energy are released when the two paired s electrons is dissociated. If metering with system energy, the E_{e-e} is a positive value, it indicates that these two electrons repel each other. For the two paired electrons in a helium atom, $E_{e-e} = I_2 - I_1 = 5250.5 - 2372.3 = 2878.2$ (KJ/mol) (here, metering it with system energy. If metering it with dissociation energy, it must be negative value).

The law expressed by Eq. (2) can be promoted to “the difference of the ionization energy of any two adjacent electrons is the interaction energy of the two electrons”. But this promotion must follow the following conditions: Before and after the ionization, the structure of the atomic core inside the two electrons is unchanged. We can use the following method to find some regular in the data of interaction energy.

The calculation method for pairing energy of free electrons

Regression analysis method is used to calculate.

(a) Lists the relation form of the difference $\Delta I(1s^2)$ of ionizing energy between two 1s electrons to the effective nuclear charge number as shown in Table 1 and Figure 1. In this paper, the interaction energy between electrons is positive in the list and the illustrations.

(b) Extracts the regression equation [$\Delta I(1s^2) = E_{e-e}(1s^2)$].

Table 1: The relations between the differences of the ionizing energy of two 1s electrons of number 1-26 elements and the nuclear charge number (unit: KJ/mol).

Elements	He	Li	Be	B	C	N	O	F
Z	2	3	4	5	6	7	8	9
$\Delta I(1s^2)$, KJ/mol	2878.20	4516.90	6157.90	7800.90	9446.00	11093.4	12748.0	14396.2
Ne	Na	Mg	Al	Si	P	S	Cl	Ar
10	11	12	13	14	15	16	17	18
16052.5	17714	19380	21050	22727	24404	26090	27766	29461
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Cu
19	20	21	22	23	24	25	26	29
31183	32912	34633	36364	38094	39863	41617	43361	48747

Table 2: Relationship between the electrons paired energy in 2s2 electron pair and the effective nuclear charge number. Energy unit is KJ/mol.

Ele.	Z	$I_{last\ 3rd}$	Z^*	$E_{e-e}(2s^2)$
Be	4	1757.1	2.31386	857.6
B	5	3659.7	3.33934	1232.6
C	6	6222.7	4.35439	1602.2
N	7	9444.9	5.36460	1969.9
O	8	13326.5	6.37230	2337.0
F	9	17868	7.37864	2703.9
Ne	10	23069.5	8.38412	3070.5
Na	11	28932	9.38918	3436
Mg	12	35458	10.3943	3805
Al	13	42647	11.3994	4174
Si	14	50502	12.4049	4540
P	15	59024	13.4107	4914
S	16	68216	14.4172	5286
Cl	17	78095	15.4259	5754
Ar	18	88576	16.4284	6103
K	19	99710	17.4304	6310
Ca	20	111711	18.4496	6811
Sc	21	124270	19.4590	7270
Ti	22	137530	20.4709	7630
V	23	151440	21.4812	8040
Cr	24	166090	22.4962	8390
M	25	181380	23.5089	8880
Fe	26	195200	24.3881	7100
Co	27	214100	25.5415	9600
Ni	28	231490	26.5586	10090
Cu	29	249660	27.5812	10560

$$\Delta I(1s^2)=E_{e-e}(1s^2)=1689.9Z-769.5. \quad (3)$$

$$\Delta I(1s^2)=E_{e-e}(1s^2)=3.1Z^2+1599.2Z-275.9, \quad (4)$$

$$\Delta I(1s^2)=E_{e-e}(1s^2)=0.0681Z^3-0.047Z^2+1638.8Z-399.73. \quad (5)$$

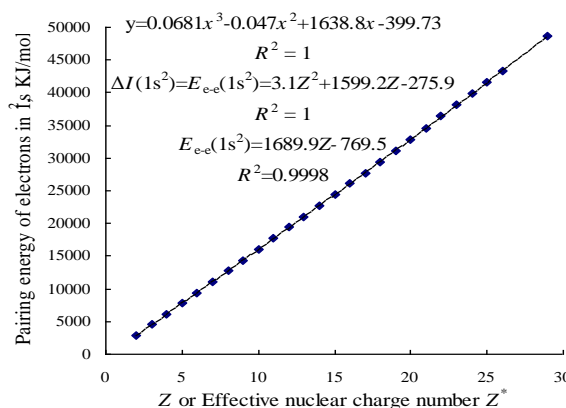


Figure 1: The relationship between the interaction energy inside the 1s² electrons and effective nuclear charge number Z* (or Z).

Using the same way to deduce Eqs. (3)-(5), we can list Table. 2 and obtain Eqs. (6) and (7) — the relationship between the electron paired energy in 2s² electron pair and the effective nuclear charge number (Eliminate the two points of Potassium element and Iron element. The figure is similar to Figure 1).

$$E_{e-e}(2s^2)=1.1178Z^{*2}+347.22Z^*+69.711. \quad (6)$$

The relationship between the atomic energy and the energy level is that the energy of the n layer is the first layer of the ground state energy (1/n²). It is believed that this relationship can be established in the calculation of the interaction energy between electrons. In the same sub layer of atoms, the energy difference of the electrons in different main layer is n² times. Therefore, if the effective nuclear charge number are the same, we have (I_{last 3rd}-I_{last 4th})=(I_{last 1st}-I_{last 2nd})/n². According to this relationship, we can promote Eq. (6). Use E_{e-e}[X(ns²)] to express the

interaction energy between the two paired-electrons outside the nuclear (their size equal mark opposite with the dissociation energy of paired electrons), promotes from $n=2$ to $n>2$ (n is principal quantum number). $E_{e-e}(2s^2)$ multiplied by 2^2 to return to the $n=1$, then divided by n^2 so as to be suitable for the case of $n \geq 2$:

$$E_{e-e}[X(ns^2)] = 2^2(1.1178Z^{*2} + 347.22Z^* + 69.711)/n^2. \quad (7)$$

This is an approximate formula, generally do not use, some of the following formula is more accurate. Although the eq. (4) is better than eq. (3) in fitting (perhaps, $e_{e-e}(1s^2) = 0.0681z^{*3} - 0.047z^{*2} + 1638.8z^* - 399.73$ is better than others). The relationship between the interaction energy of electron-electron and the number of nuclear charge may be linear. The difference between the two equations may root in the ionization energy data and the drawing tool. We have no good reason to say eq. (4) is not set up. So, the three formulas are used by me. I will list them and their promotion, which will be chosen by the readers. For molecules, the z^* in eqs. (6) and (7) may be σz^* . In order to confirm the accuracy of eq. (4), substituting $z^* = 11$ into eq. (4), results in $e_{e-e}[\text{na}(1s^2)] = 17690.4 \text{ kJ/mol}$. The experimental value is the difference between i_{10} and i_{11} of sodium element: $i_{11} - i_{10} = 17714.0 \text{ mJ/mol}$. When $z^* = 0$ and $n = 1$, $e_{e-e}(1s^2) = -275.9 \text{ mJ/mol}$ is the pairing energy of two free electrons. It can be expressed by δ . That is, the pairing energy of free electron is $\delta = -275.9 \text{ kJ/mol}$. This pairing energy is very useful in superconductor theory. A principle and method for measurement of the electron pairing energy is obtained when eqs. (1)-(7) are obtained. Experimental method corresponding to this experiment principle is measurement of the interaction energy between electrons with the method of measuring ionization energy.

The relationship between the pairing energy in $2s^2$ electrons and the number of nuclear charge and the atomic number

Applying Eqs. (6) and (7) to calculate ns^2 ($n \geq 2$) electron pair, the results have errors, the error sources have: the error of calculation results of effective nuclear charge number; the error of ionization energy data; the defect of constructing tool. It is necessary to find out the law of the interaction energy between $2s^2$ electrons directly.

We calculate the effective nuclear charge acting on the $2s^2$ electron according to the last third ionization energy: $I_{\text{last } 3\text{rd}} = 1312.75 (Z^*)^2/2^2$ (similarly hereinafter). This algorithm does not consider the size effect of the atomic kernel, and has some errors. We can calculate $\Delta I(2s^2)$ according to the Eq. (2). The calculation results are shown in the 4th column in Table 2.

The linear regression equation is obtained according to the data in Table 3.

$$E_{e-e}(2s^2) = 371.69Z - 639.24. \quad (8)$$

The method to extend Eq. (8) to the ns^2 : Eq. (8) multiplied by 2^2 , so that it applies to $1s^2$ electronics, and then divided by n^2 .

$$E_{e-e}(ns^2) = (371.69Z - 639.24) \times 2^2/n^2. \quad (9)$$

Similarly, the relationship between energy and the effective nuclear charge number Eq. (5) can be obtained by applying Table S1.

$$E_{e-e}(2s^2) = 364.75Z^* + 13.386, \quad (10)$$

$$E_{e-e}(2s^2) = 0.1181Z^{*2} + 363.13Z^* + 17.954. \quad (11)$$

Note: eqs. (10) and (11) is a simplified form of eqs. (6) and (7); eqs. (8) and (9) are completely different from eqs. (6) and (7), do not mix. In the application process, the use of eqs. (8) and (9) calculation is simpler. If you can only use the effective nuclear charge, we have to use eqs. (10) and (11) or eqs. (6) and (7). If it is used for the calculation of molecules, the eqs. (6), (7), (10) and (11) are more useful than eqs. (8) and (9).

The relationship between the interaction energy of two Spin-parallel $2p$ electrons and the unclear charge number

When an element is ionized, and the second layer is left with two $2p$ electrons, the two $2p$ electrons are in the same spin as the non pairing state [expressing it with $2p^{\uparrow\uparrow}$ or $p^{\uparrow\uparrow}(\text{in } 2p^2)$]. Using above train of thought, the following formula can be summed up.

$$E_{e-e}(p^{\uparrow\uparrow})(\text{in } 2p^2) = \Delta I(2p^{\uparrow\uparrow}) = (I_{\text{last } 5\text{th}} - I_{\text{last } 6\text{th}}). \quad (12)$$

According to Eq. (12), the calculation results are shown in the 7th column in Table 3. The linear regression equation is obtained according to nuclear charge number and the data shown in the 7th column in Table 3 (shown in Fig. 2).

$$E_{e-e}(p^{\uparrow\uparrow})(\text{in } 2p^2) = 455.6Z - 1495.7, \quad (13)$$

According to $E_{e-e}(p^{\uparrow\uparrow})(\text{in } 2p^2)$ calculate the average distance between the two single $2p^{\uparrow}$ electrons. The interaction energy increases with the increase of the effective nuclear charge number, the average distance between electrons is smaller and smaller, the distance between the $2p$ electron and the nucleus is also getting smaller and smaller.

When an atom is ionized only three $2p$ electrons are left, the interaction energy between the three spin-parallel $2p$ electrons is $E_{e-e}(p^{\uparrow\uparrow})(\text{in } 2p^3) = I_{\text{last } 6\text{th}} - I_{\text{last } 7\text{th}}$. The data of $E_{e-e}(p^{\uparrow\uparrow})(\text{in } 2p^3)$ of Nitrogen like ion are shown in the 8th column in Table 2. Using the same method, we can obtain

$$E_{e-e}(p^{\uparrow\uparrow})(\text{in } 2p^3) = 459.9Z - 1798.2. \quad (14)$$

If the number of nuclear charges replaced by the effective nuclear charge number as in Table S2, Eq. (15) can be

obtained. $E_{e-e}(p^{\uparrow\uparrow})(in 2p^3)=1.5382Z^{*2}+416.77Z^*+144.71$ and the number of effective nuclear charge are beneficial
 (15). All relationship between electron interaction energy to the calculation of the molecules.

Table 3: The relationship between “the interaction energy of electron-electron” and the number of nuclear charge (energy unit: KJ/mol).¹

Elements↓	Z↓	$E_{e-e}(1s^2-2s^1)$	$E_{e-e}(2s^2)=\Delta I(2s^2)$	$E_{e-e}(1s^2-2p^1)$	$E_{e-e}(2s^2-2p^1)$	$E_{e-e}(p^{\uparrow\uparrow})(in 2p^2)$	$E_{e-e}(p^{\uparrow\uparrow})(in 2p^3)$	$E_{e-e}(p^{\uparrow\downarrow})(in 2p^4)$	$E_{e-e}(p^{\uparrow\downarrow})(in 2p^6)$
Li	3	2433.5							
Be	4	3493.9	857.6						
B	5	4545.0	1232.6						
C	6	5592.1	1602.2	1892.4	7569.7	1266.1			
N	7	6636.3	1969.9	2300.6	9202.5	1722.1	1453.7		
O	8	7677.6	2337.0	2707.0	10827.9	2168.7	1912.2	2074.4	
F	9	8715.3	2703.9	3112.1	12448.5	2615.0	2357.3	2676.2	
Ne	10	9749.4	3070.5	3516.2	14064.7	3056.0	2806	3249	2727.2
Na	11	10778.8	3436	3918.8	15675.0	3504	3259	3811	3221.1
Mg	12	11801.1	3805	4319.6	17278.5	3950	3691	4390	3716.6
Al	13	12816.9	4174	4722.2	18888.7	4388	4139	4947	4200.0
Si	14	13822.9	4540	5119.8	20479.2	4848	4591	5507	4689.7
P	15	14818.4	4914	5446.5	21785.9	5311	5045	6033	5169.3
S	16	15800.3	5286	5911.3	23645.0	5750	5533	6556	5639.3
Cl	17	16751.5	5754	6296.7	25186.8	6244	6051	7107	6115.7
Ar	18	17757.1	6103	6683.0	26732.1	6719	6546	7651	6598.7
K	19	18766.0	6310	7079.2	28316.8	7180	6950	8220	7093.3
Ca	20	19564.4	6811	7455.1	29820.3	7690	7420	8780	7590.0

Table S1: The relationship between Ee-e(2s²) and effective nuclear charge number Z*.

Elements	Be	B	C	N	O	F	Ne	Na	Mg	Al
Z*	2.3139	3.3394	4.3544	5.3646	6.3724	7.3787	8.3842	9.3893	10.3944	11.3994
$E_{e-e}(2s^2)=\Delta I(2s^2)$	857.6	1232.6	1602.2	1969.9	2337	2703.9	3070.5	3436	3805	4174
$E_{e-e}(1s^2-2s^1)$	3493.9	4545	5592.1	6636.3	7677.6	8715.3	9749.4	10778.8	11801.1	12816.9

Table S2: The relationship between Ee-e(2p^{↑↑})(in 2p²) and effective nuclear charge number Z*.

Elements	C	N	O	F	Ne	Na	Mg	Al	Si	P
Z*	2.6674	3.73495	4.7707	5.7954	6.8141	7.8293	8.8426	9.8518	10.8328	11.8726
$E_{e-e}(p^{\uparrow\uparrow})(in 2p^2)$	1266.1	1722.1	2168.7	2615.0	3056.0	3504	3950	4388	4848	5311

Table S3: The coefficient matrix of the assemblage of energy equation of the carbon-like ions.

Terms	Z ²	Z	Z ⁰
$2E_{n-e}(1s^1)$	-2625.508	0	0
$2E_{n-e}(2s^1)$	-656.377	0	0
$2E_{n-e}(2p^1)$	-656.377	0	0
$E_{e-e}(1s^2)$	3.1	1599.2	-275.9
$E_{e-e}(2s^2)$	0	371.69	-639.24
$E_{e-e}(p^{\uparrow\uparrow})(in 2p^2)$	0	455.6	-1495.7
$2E_{e-e}(1s^2-2s^1)$	0	2045.2	-1074.88
$2E_{e-e}(1s^2-2p^1)$	0	794.78	-934.8
$2E_{e-e}(2s^2-2p^1)$	0	3179.12	-3739.2
Σ	3938.262	8445.59	-8159.72

Table S4: The coefficient matrix of the assemblage of energy equation of the neon-like ions.

Terms	Z ²	Z	Z ⁰
2E _{n-e} (1s ¹)	-2625.508	0	0
2E _{n-e} (2s ¹)	-656.377	0	0
6E _{n-e} (2p ¹)	-1969.131	0	0
E _{e-e} (1s ²)	3.1	1599.2	-275.9
E _{e-e} (2s ²)	0	371.69	-639.24
12E _{e-e} (p [↑] ↑)(in 2p ²)	0	5518.8	-21578.4
3E _{e-e} (p [↑] ↓)(in 2p ⁶)	0	1451.7	-6295.8
2E _{e-e} (1s ² -2s ¹)	0	2045.2	-1074.88
6E _{e-e} (1s ² -2p ¹)	0	2384.34	-2804.4
24E _{e-e} (2s ² -2p ¹)	0	9537.36	-11217.6
Σ	-5247.916	22908.29	-43886.22

The relationship between “the interaction energy between 2s¹ electron and 1s² electrons” and the number of nuclear charge

The symbols of positive-negative are easy to mistake, therefore. Note! E_{n-e} is negative; E_{e-e} is positive, or we meter some terms with absolute value at an appropriate time. The interaction energy between 2s¹ electron and 1s² electrons is equal to |2E_{n-e}(1s¹)+E_{n-e}(2s¹)|-ΣI_{last 1st-3rd} (the absolute value of the differences between the sum of the energies of the Schrodinger equations and the sum of the ionization energy of the three electrons) again subtracts E_{e-e}(1s²) (the paired energy of 1s²):

$$E_{e-e}(1s^2-2s^1) = -(I_{last\ 1st} + I_{last\ 2nd} + I_{last\ 3rd}) - 2E_{n-e}(1s^1) - E_{e-e}(1s^2) - E_{n-e}(2s^1) \tag{16}$$

If does not consider relativistic effect, its value is E_{n-e}(2s¹)=Z²E_H/n²=-13.606Z²/n². The case of E_{n-e}(2p¹) is also the same. Considering E_{e-e}(1s²)=ΔI(1s²)=I_{last 1st}-I_{last 2nd}, both 2E_{n-e}(1s¹) and E_{n-e}(2s¹) are negative, Eq. (16) becomes

$$E_{e-e}(1s^2-2s^1) = -2E_{n-e}(1s^1) - E_{n-e}(2s^1) - (I_{last\ 1st} + I_{last\ 2nd} + I_{last\ 3rd}) - I_{last\ 1st} + I_{last\ 2nd} \\ = -2E_{n-e}(1s^1) - E_{n-e}(2s^1) - 2I_{last\ 1st} - I_{last\ 3rd}$$

If the relative effects are all considered, I_{last 1st} is equal to -E_{n-e}(1s¹), result in

$$E_{e-e}(1s^2-2s^1) = |E_{n-e}(2s^1)| - I_{last\ 3rd} \tag{17}$$

Where, the interaction of I_{last 3rd} requires the nucleus and the 1s² electrons, yet E_{n-e}(2s¹) is only the interaction between 2s¹electron and the nucleus. Thus, |E_{n-e}(2s¹)|-I_{last 3rd} is the interaction energy between 2s¹electron and 1s² electrons. The first item on the left in Eq. (17) is the theoretical result of quantum mechanics. It determines that Eq. (17) is the quantum mechanical method. The interaction energy between 1s² electrons and two 2s¹ electrons is multiply the 2E_{e-e}(1s²-2s¹):

$$E_{e-e}(1s^2-2s^2) = 2E_{e-e}(1s^2-2s^1) = 2[|E_{n-e}(2s^1)| - I_{last\ 3rd}] \tag{18}$$

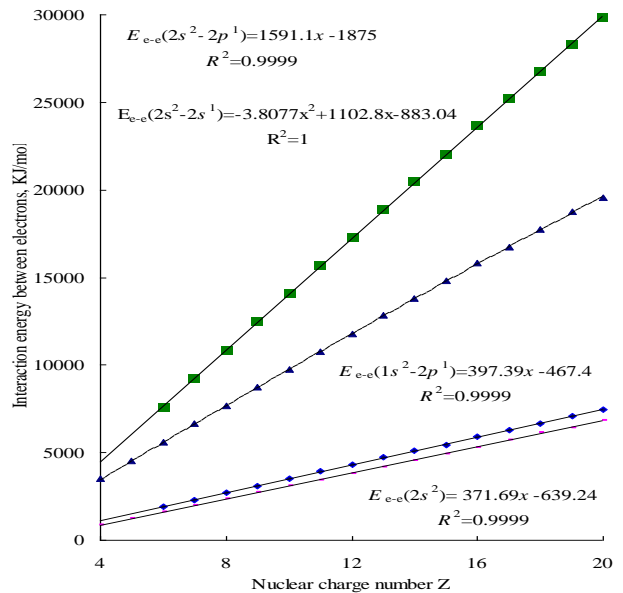


Figure 2: The relationship between the interaction energy of the electrons in 2nd layers and the nuclear charge number.

Taking lithium atom as an example, the interaction between 2s¹ and 1s² is E_{e-e}(1s²-2s¹)=|E_{n-e}(2s¹)|-I_{last 3rd}=2952.0-520.2=2431.8 (KJ/mol).

The data of Li-like ion obtained by according to Eq. (17) are listed in the 3rd column in Table 3. The linear regression equation is obtained according to the nuclear charge number and the data in the third column in Table 3.

$$E_{e-e}(1s^2-2s^1) = 1022.6Z - 537.44, \text{ (Elements 3-18); } \tag{19}$$

$$E_{e-e}(1s^2-2s^1) = -3.1394Z^2 + 1088.5Z - 816.86, \text{ (Elements 3-18). } \tag{20}$$

The relationship between $E_{e-e}(1s^2-2s^1)$ and the number of effective nuclear charge can be obtained by according to the data in Table S1 in Supplementary materials:

$$E_{e-e}(1s^2-2s^1)=1027.7Z^*+1121, \quad (21)$$

$$E_{E-E}(1S^2-2S^1)=-1.0692Z^{*2}+1042.4Z^*+1079.6. \quad (22)$$

The relationship between “the interaction energy between $2p^1$ electron and $2s^2$ electrons” and the number of nuclear charge

Considering Eq. (17), the relationship between this interaction energy and ionization energy is that the interaction energy between a $2p^1$ electron and the inside of four electrons ($1s^2$ and $2s^2$) minus the interaction energy between $1s^2$ and $2p^1$:

$$E_{e-e}(2s^2-2p^1)=|E_{n-e}(2p^1)|-I_{last\ 5th}-|E_{e-e}(1s^2-2p^1)|,$$

and

$$E_{e-e}(1s^2-2p^1)=E_{e-e}(2s^2-2p^1)/2^2. \quad (23)$$

Considering Eq. (23), $E_{e-e}(2s^2-2p^1)=|E_{n-e}(2p^1)|-I_{last\ 5th}-|E_{e-e}(1s^2-2p^1)|$ becomes

$$E_{e-e}(1s^2-2p^1)=\{|E_{n-e}(2p^1)|-I_{last5th}\}/(2^2+1); \quad (24)$$

$$E_{e-e}(2s^2-2p^1)=2^2\{|E_{n-e}(2p^1)|-I_{last5th}\}/(2^2+1). \quad (25)$$

Where, $E_{n-e}(2p^1)=-1.31275Z^2/n^2$. The data in the 5th column and 6th column in Table 3 can be drawn by applying the data of ionization energy and Eqs. (23)-(25). The linear regression equation is obtained according to the data in 5th column in Table 3.

$$E_{E-E}(1S^2-2P^1)=397.39Z-467.4. \quad (26)$$

The relationship between “the interaction energy inside $2p^{\uparrow\downarrow}$ electrons” and the number of nuclear charge

After the $2p^4$ electrons Oxygen atom or oxygen-like cores losing two electrons, the configuration of $2p$ electrons from $2p^{\uparrow\downarrow}-2p^{\uparrow}-2p^{\uparrow}$ comes into $2p^{\uparrow}-2p^{\uparrow}-2p^0$. A $2p^{\uparrow\downarrow}$ electron pair is destroyed, without increasing the single electron. It is accordance with the condition of promotion of Eq. (2).

$$E_{e-e}(p^{\uparrow\downarrow})(in\ 2p^4)=\Delta I(2p^{\uparrow\downarrow})=I_{last7th}-I_{last8th}. \quad (27)$$

This is the rules of electron paired energy in $2p^4$ electrons configuration. It can be extended to the case of $n>2$. For oxygen atom, according to Eq. (27), the calculation result is 2074.4KJ/mol. Under Eq. (27) we can list the data in the 9th column in Table 3) and Eq. (28).

$$E_{e-e}(p^{\uparrow\downarrow})(in\ 2p^4)=554.2Z-2297.3. \quad (28)$$

Here, “in $2p^{4n}$ ” express that $p^{\uparrow\downarrow}$ is an electronic pair of the arrangement in $2p^4$.

After $2p^5$ in a Fluorine atom or an atomic kernel of Fluorine-like lose two electrons, the electron arrangement of $2p$ electrons change into $2p^{\uparrow}-2p^{\uparrow}-2p^{\uparrow}$ from $2p^{\uparrow\downarrow}-2p^{\uparrow\downarrow}-2p^{\uparrow}$. The two $2p^{\uparrow\downarrow}$ electron pair have been destroyed; two single electrons have been added. It does not conform to the popularization condition of Eq. (2). In this case the electronic pairing energy can be temporarily unable to calculate directly. We can calculate the energy of the Fluorine atom and the Fluorine-like atomic kernel by means of the method to will introduce. After the total energy of a Fluorine atom is calculated, We can deduce $E_{e-e}(p^{\uparrow\downarrow})(in\ 2p^5)$.

After $2p^6$ in a atom or an atomic kernel lose two electrons, the arrangement of $2p$ electrons changes into $2p^{\uparrow\downarrow}-2p^{\uparrow}-2p^{\uparrow}$ from $2p^{\uparrow\downarrow}-2p^{\uparrow\downarrow}-2p^{\uparrow\downarrow}$. The two $2p^{\uparrow\downarrow}$ electron pair have been destroyed; two spin parallel electrons have been added. Although it does not conform to the popularization condition of Eq. (1), but there are other rules to follow. If the arrangement of $2p$ electrons in an atomic core is $2p^{\uparrow\downarrow}-2p^{\uparrow\downarrow}-2p^0$, $I_{last\ 10th}-I_{last\ 9th}$ is the imaginary electronic pairing energy. It needs to add a pair $2p^{\uparrow\downarrow}$ electron and reduces two electrons when the arrangement of $2p$ electrons in the atomic core restores to $2p^{\uparrow\downarrow}-2p^{\uparrow\downarrow}-2p^0$ from $2p^{\uparrow\downarrow}-2p^{\uparrow}-2p^{\uparrow}$. The variation of the corresponding interaction energy is $E_{e-e}(2p^{\uparrow\downarrow})-E_{e-e}(2p^{\uparrow\uparrow})$. In this way, we have: $\Delta I(2p^{\uparrow\downarrow})_{2\ pairs\ of\ electrons}=2E_{e-e}(2p^{\uparrow\downarrow})-E_{e-e}(2p^{\uparrow\uparrow})$.

$$E_{e-e}(2p^{\uparrow\downarrow})_{2\ pairs\ of\ electrons}=[\Delta I(2p^{\uparrow\downarrow})+E_{e-e}(2p^{\uparrow\uparrow})]/2=(I_{last\ 9th}-I_{last\ 10th}+I_{last\ 5th}-I_{last\ 6th})/2. \quad (29)$$

This is the average value of two pairs $2p^{\uparrow\downarrow}$ electrons which were separated. The rest of the $2p^4$ lost two electrons, which can be calculated by Eq. (18): $E_{e-e}(2p^{\uparrow\downarrow})=\Delta I(2p^{\uparrow\downarrow})=I_{last\ 7th}-I_{last\ 8th}$. The average pairing energy of 3 pair electrons in $2p^6$ is

$$E_{e-e}(p^{\uparrow\downarrow})(in\ 2p^6)=[\Delta I(2p^{\uparrow\downarrow})+E_{e-e}(2p^{\uparrow\uparrow})]/3 \\ =[(I_{last\ 9th}-I_{last\ 10th})+(I_{last\ 7th}-I_{last\ 8th})+(I_{last\ 5th}-I_{last\ 6th})]/3. \quad (30)$$

According to Eq. (30), we can obtain the data in 10th column in Table 3 and Eq.(31).

$$E_{e-e}(p^{\uparrow\downarrow})(in\ 2p^6)=483.9Z-2098.6. \quad (31)$$

Exploration of mechanism of electron pairing

Previously only know that there is a similar attraction between proton and proton. Since the existence of short-range stronger electromagnetic force between electrons, then electron pairing is actually overlap. There also is stronger attraction between electrons. Whether its nature is the complete same with the one between protons? This problem also needs to explore. The authors consider they are the same. They are all short-range forces, the strength have something to do with the size of the free particle — the smaller the size, the greater the intensity. Reveal deeper mechanisms need to be completed by everybody.

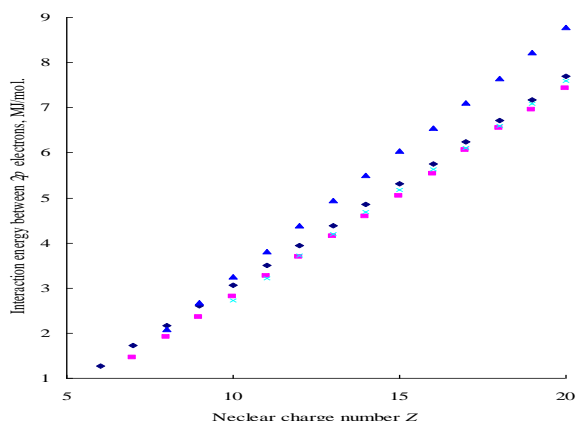


Figure 3: The relationship between the interaction energy of 2p electrons and nuclear charge number.

There is stronger attraction between electrons when they are very close or overlapping. It shows that an electron is not a point particle. When the electromagnetic interaction is discussed, the classical electromagnetic theory takes charge as a point particle.

The non point particle is not in conformity with the classical electromagnetic theory necessarily. Since the short-range stronger of strong attraction between like charges is widespread, the infinite interaction between like charges to be very near would not exist. So, the problem of energy divergence does not exist. Electron has both the characteristic of non-point and the one to can be overlapped. It can express that the electron is wave in essence. In the process of the experiment, it is easy to realize the mutual transformation between electron and electromagnetic wave.

The exploration of the above shows that here exploration on the nature of the electronic structure and the interaction between the electron and the electron is the grow point of new theory.

On the study of the nature of the interaction energy between electrons can make that this manuscript contains the sort of significant conceptual advance in understanding or methodology that will be of immediate interest to a broad readership of researchers in the physics community.

The calculation method for interaction energy between elements and its application

This is also the law of the relationship between “atomic energy and atomic core energy” and “ionization energy and atomic number”& their application.

Eqs. (3)-(7), (10)-(11), (13)-(15), (19)-(22), (26)-(27), (28) and (31) are the results of the statistics. In this section, we will continue to introduce some of the results

of regression statistics and apply them to the calculation of the energy of atoms and ions. First, we introduce a small application to be not important, and then introduce important applications.

Correction of the effective nuclear charge number, check the ionization energy data

The number of effective nuclear charge experienced by the outer layer electron is always an estimate value. This is very bad for the calculation of the valence electrons. As long as the data of ionization energy is accurate, the effective nuclear charge number can be very accurately calculated by according to the statistical law of this paper.

Substituting the relationship between a ionization energy of Mg element and electron pairing energy $I_{11}-I_{12}=713.00=E_{e-e}(3s^2)$ into $E_{e-e}(3s^2)=(0.0681Z^{*3}-0.047Z^{*2}+1638.8Z^*-399.73)/3^2$, can obtain $Z^*(Mg^{2+})=4.1574$ the effective nuclear charge number for 3s electrons. According to the relation of $I_2=Z^{*2}/n^2$, the calculated value is 3.1537. J. C. Slater experience is 3.2. To make sure that this correction is meaningful, must improve the accuracy of the measurement of ionization energy.

The calculation results of $|e_{n-e}(2s^1)|-i_{last\ 3rd}$ have a certain rule. But iron element has a large deviation. It is estimated that $i_{last\ 3rd}$ of fe is incorrect (should not be 195200kj/mol and should be 197400kj/mol or so). $E_{e-e}(2s^2)-z$ curve can be drawn by according to the data in Table 2. The point of 19th element also deviates from the fitting of the straight line. It is estimated that the $i_{last\ 3rd}$ or $i_{last\ 4th}$ of the k element is incorrect (their difference should be about 6410kj/mol, not 6310kj/mol).

Development of new quantum mechanics calculation method: regression equation method (or fitting curve method)

One by one calculation of electronic energy and the interaction energy between electrons

(a) The energy of the negative hydrogen ion and helium atom

Substituting $Z=1$ and $n=1$ into Eq. (5), a negative hydrogen ion energy can be obtained: $E[H^-(1s^2)]=2E_{n-e}(H)+E_{e-e}[H(1s^2)]=-2624.0+1239.09=-1384.9$ (KJ/mol). It is slightly lower than the energy of a ground state hydrogen atom, and shows that this system has certain stability.

According to Eq. (5), We can also calculate the ground state energy of helium atom conveniently: $E_{e-e}(He)^{(0)}=E_{n-e}(He)+E_{e-e}[He(1s^2)]=-10502.00KJ/mol+ 2878.23 KJ/mol=-7623.77 KJ/mol$. Relative error is $(7623.77-7622.8)/7622.8=0.0013\%$.

(b) The energy of the Lithium atom and the energy of the Beryllium atom

The energy of the ground state lithium atom=(the interaction energy between the two 1s electrons and the nuclear)+(the interaction energy between a 2s electron and the nuclear)+(the interaction energy between the two 1s electrons)+(the interaction energy between the 1s² electrons and 2s¹ electron). The calculation in front of the two terms is relatively simple. The calculation of following two terms are respectively based on Eq. (5) and Eqs. (19) and (20) to calculate (Don't need ionization energy data, directly substituting Z=3 into the two regression equation). The calculation results are:

$$E(\text{Li})^{(0)} = -2 \times 3^2 \times 1312.75 - 3^2 \times 1312.75/2^2 + 4518.09 + 2443.93$$

$$= -23629.6 - 2953.70 + 4518.09 + 2443.93$$

$$= -19621.3 \text{ (KJ/mol)}$$

The corresponding experimental value is -19633.3KJ/mol. The relative error is 0.06%. More computational examples see first calculation method of carbon, nitrogen and neon in the next section.

Transverse regression analysis method for each element spread along the atomic cores

Eqs. (3)-(5) is suitable for the calculation of the energy of the 1s² elements in all atoms. Referring to the lithium atom, the energy of the ground state carbon atom is

$$E(\text{C})^{(0)} = 2E_{n-e}(1s^1) + 2E_{n-e}(2s^1) + 2E_{n-e}(2p^1) + E_{e-e}(1s^2) + E_{e-e}(2s^2) + 2E_{e-e}(1s^2-2s^1) + E_{e-e}(2p^{\uparrow\uparrow}) + 2E_{e-e}(1s^2-2p^1) + 2E_{e-e}(2s^2-2p^1) \quad (32)$$

The calculation in front of the three terms is relatively simple (establish the potential energy function and Schrodinger equation for the hydrogen like ions, then calculation of them. This is also standard, basic quantum mechanics theory method). Use Eq. (4) to calculate E_{e-e}(1s²), Use Eq. (8) to calculate E_{e-e}(2s²), Use Eq. (20) to calculate E_{e-e}(1s²-2s¹), Use Eqs. (13) and (14) to calculate E_{e-e}(2p^{↑↑}), Use Eq. (26) to calculate E_{e-e}(1s²-2p¹), Use Eq. (23) and Eq. (26) to calculate E_{e-e}(2s²-2p¹). Result in E(C)⁽⁰⁾ = -99263.7 (MJ/mol). The experimental value is -99390.3 MJ/mol. The relative error is 0.13%. The calculation of the each term in Eq. (32) is based on an equation which has only Z of the independent variable. They can be set for a coefficient matrix of 3 columns of 9 lines as given in Table S3. Thus, a combined formula of calculation can be obtained:

$$E(\text{Carbon-likeion})^{(0)} = -3938.262Z^2 + 8434.99Z - 8042.96 \quad (33)$$

Summing up Eq. (33) is more troublesome. In practice, this method is generally not used. However, the process of deriving Eq. (33) can tell us about the specific circumstances of the interaction between electrons. A regression equation can be obtained by using the 8 data in front of Si in the 5th column in Table 4.

$$-E(\text{C-likeion})^{(0)} = -\Sigma I(\text{C-likeion}) = 2.6Z^3 + 3896.7Z^2 - 8376.5Z + 8805.1, \text{ (8 points)} \quad (34)$$

Add 16 elements (see the 5th column in table 4) to get the Eq. (35).

$$-E(\text{C-likeion})^{(0)} = -\Sigma I(\text{C-likeion}) = 3.9Z^3 + 3.8298Z^2 - 7426.5Z + 4918.4, \text{ (24 points)} \quad (35)$$

Eq. (33) is more close to Eq. (34). It indicates that, in this paper, the analytical methods and results about the interaction of electrons in atoms are correct basically. At least, it can indicate that the research directions of the interaction energy between electrons in atom are correct. The difference between Eq. (33) and Eq. (34) reminds us: The error of the ionization data must be further reduced; Calculation of the interaction energy between electrons must be more careful; Better drawing tools should be used; Relativistic effects cannot be considered. If there is no the inference process of deriving Eq. (33), we don't know that the quadratic term in Eq. (34) is the interaction energy between electrons and nuclear, both the first power term and the constant term in Eq. (34) are the interaction energy between electrons. The energy of Carbon atoms obtained by directly using Eq. (35) is -99074.6KJ/mol. The relative error is 0.3%. these Carbon-like ions N⁺, O²⁺, F³⁺ and Ne⁴⁺ and so on, can also be calculated by means of the same method..

The calculation of Neon atom is the same as the Carbon atom, only the coefficients of the terms of the interaction energy involved 2p electron should be changed.

$$E(\text{Ne})^{(0)} = 2E_{n-e}(1s^1) + 2E_{n-e}(2s^1) + 6E_{n-e}(2p^1) + E_{e-e}(1s^2) + E_{e-e}(2s^2) + 2E_{e-e}(1s^2-2s^1) + [12E_{e-e}(2p^{\uparrow\uparrow}) + 3E_{e-e}(2p^{\uparrow\downarrow})] + 6E_{e-e}(1s^2-2p^1) + 6E_{e-e}(2s^2-2p^1) \quad (36)$$

Where, The item of 3E_{e-e}(2p^{↑↓}) cannot be calculated by the formula of the electron pairing energy in 2p⁴, which should be calculated according to Eq. (31), the value is 8221.2KJ/mol. We use Eq. (4) to calculate E_{e-e}(1s²), use Eq. (8) to calculate E_{e-e}(2s²), use Eq. (8) to calculate E_{e-e}(2s²), the results were as follows: 16026.1 KJ/mol and 3077.66KJ/mol. We use Eq. (20) to calculate 2E_{e-e}(1s²-2s¹), the result is 19508.4KJ/mol. We use Eq. (26) to calculate 6E_{e-e}(1s²-2p¹), the result is 21039KJ/mol. We use Eqs. (23) and (26) to calculate 6E_{e-e}(2s²-2p¹), the result is 84156 KJ/mol. We use Eq. (14) to calculate 12E_{e-e}(2p^{↑↑}), the result is 33609.6KJ/mol. The first three terms in Eq. (36) are calculated by according to quantum mechanics theory method, the result is -525101.6KJ/mol. Substitute these results into Eq. (36), result in E(Ne)⁽⁰⁾ = -339473.7KJ/mol. The relative error is 0.2%. The energy of the sum of the ionization energies does not represent the experimental values of the ground state Neon atom. Because, after the first electron, second electron and third electron ionizes, the interior of the atoms are all electronic rearrangement. In the process of the electronic rearrangement, the energy exchange between the atomic core and the environment occurs. This is the author's understanding of the calculation of the energy of Neon

atom. The conclusion of "the sum of the ionization energy is not necessarily equal to the total energy of the atom" is the other significance to explore the calculation method of Neon atom. The energy of Neon-like ions of ground state all can be calculated by using Eq. (36).

The calculation of the each term in Eq. (36) is based on an equation which has only Z of the independent variable. They can be set for a coefficient matrix of 3 columns of 10 lines as shown in Table S4. Thus, a combined formula of calculation can be obtained:

$$E(\text{Neon-like ion}) = -\Sigma I(\text{Neon-like ion}) = -5247.916Z^2 + 22908.29Z - 43886.22. \quad (37)$$

A group of data of the nuclear charge number and energy of the Ne like ion are listed in the 7th Column in Table 4. Drawing of them for atomic number can obtain the regression equation for this set of data as shown in Figure 4.

$$-E(\text{Neon-like ion})^{(0)} = \Sigma I(\text{Neon-like ion}) = 303.3Z^2 - 24185Z + 50318, \quad (6 \text{ points}). \quad (38)$$

Add 14 elements to get the Eq. (39).

$$-E(\text{Neon-like ion})^{(0)} = \Sigma I(\text{Neon-like ion}) = 5463.3Z^2 - 29593Z + 91091, \quad (20 \text{ points}). \quad (39)$$

According to Eqs. (37)-(39), the energy of Neon-like ions can be easily calculated (energy unit: KJ/mol). The energy of Mg^{2+} is calculated by using Eq. (39) result in -522690.2 KJ/mol . The experimental value is -523764.2 KJ/mol . The relative error is 0.2%. Eq. (37) is relatively close Eq. (38). It shows that the analytical methods and results about the interaction between electrons in atom or molecule in this paper are correct, once again.

Readers can experience above two calculation methods taking Nitrogen atom as an example. The calculation of ground state Nitrogen atom is the same as the carbon atom:

$$E(N)^{(0)} = 2E_{n-e}(1s^1) + 2E_{n-e}(2s^1) + 3E_{n-e}(2p^1) + E_{e-e}(1s^2) + E_{e-e}(2s^2) + 2E_{e-e}(1s^2-2s^1) + 3E_{e-e}(2p^{\uparrow 1}) + 3E_{e-e}(1s^2-2p^1) + 3E_{e-e}(2s^2-2p^1). \quad (40)$$

ΣI (N-like ion) values in the 6th column in Table 4 are available for use. Drawing of the values for atomic numbers result in:

$$-E(\text{N-like ion})^{(0)} = 4310.2Z^2 - 12215Z + 17751, \quad (12 \text{ points}); \quad (41)$$

$$-E(\text{N-like ion})^{(0)} = 4033.3Z^2 - 10655Z + 19858, \quad (23 \text{ points}). \quad (42)$$

Substituting the atomic number (also is nuclear charge number) into Eq. (41) or Eq. (42), you can obtain the energy of Nitrogen atom.

Longitudinal regression analysis method of atomic energy

This method can be divided into two kinds of situations, such as piecewise fitting and non-subsection fitting.

(a) Longitudinal piecewise regression analysis by period

Drawing of the data in 8th column in Table 4 for atomic number z , fig. 5 can be obtained (the fitting situation of its curve shown in fig. 6). Figure 6 shows that the best piecewise fit by the period. The sum of the interaction energy between the electrons and the nuclear in atom is $\sigma z^2/n^2$.

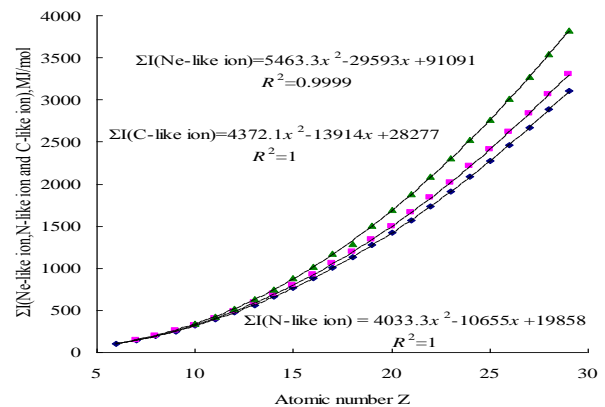


Figure 4: The relationship between the ion energy of "nitrogen-like, carbon-like neon-like" and nuclear charge number (or atomic number).

The sum of ionization energy in an atom is σi . The data in the 8th column in Table 4 is the difference of them. For the ground state atom in second periodic elements, drawing of $\Sigma Z^2/n^2 - \Sigma I$ Fig. 6 and Eq. (43) can be obtained.

$$E_{e-e} \text{ (in atom)} = 182.98Z^3 - 21.137Z^2 + 462.9x + 806.91, \quad (\text{Elements 3-10}); \quad (43)$$

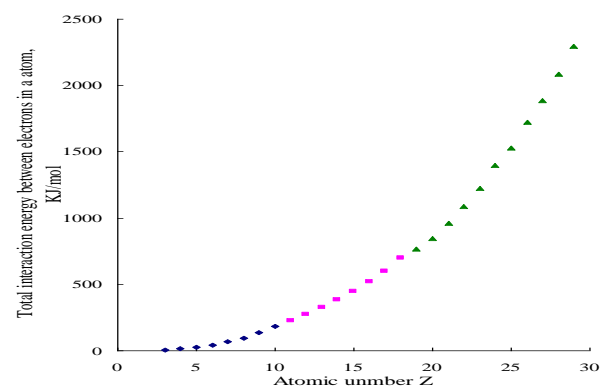


Figure 5: The relationship between the interaction energy of electron-electron in atoms and atomic number.

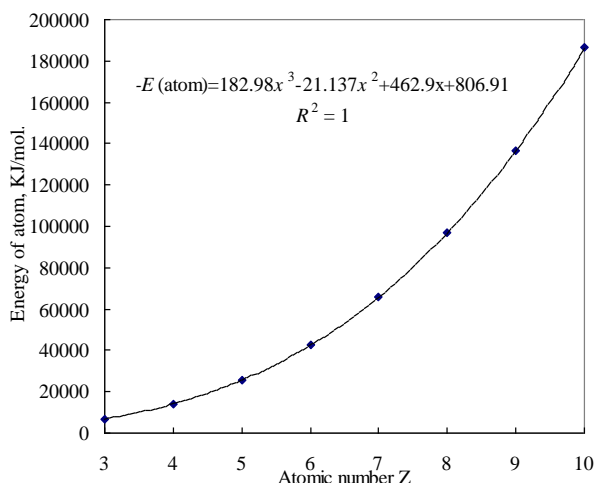


Fig. 6. The relationship between the interaction energy of electron-electron the atoms in 2nd period and atomic number.

The energy of an atom equals the sum of total energy of the atom and interaction energy of electron-electron. For verification, we take nitrogen and oxygen as the example. Substituting $z=7$ into eq. (43), result in $e_{e-e}(n)^{(0)}=62762.14-1035.713+3240.3+806.91=65773.3$ (kj/mol). Substituting $z=8$ into eq. (43), result in $e_{e-e}(o)^{(0)}=93685.76-1352.768+3703.2+806.91=96843.1$ (kj/mol). $E(\text{atom})^{(0)}=-\sigma z^2/n^2+(\text{the sum of interaction energy between electrons in an atom})$. The energy of the ground state nitrogen atom and oxygen atom respectively are: $e(n)^{(0)}=-209056.1+65773.3=143282.8$ (kj/mol). The experimental value is -143382.9 kj/mol, the relative error is 0.07%.

$E(O)^{(0)}=-294057.0+96843.1=-197213.9$ (KJ/mol). The experimental value is -197195.9 KJ/mol, the relative error is 0.01%.

Use the same method to dispose the atoms of the elements in 3rd period and 4th period, we have:

$$E_{e-e}(\text{in atom})=0.2012Z^3-4.838Z^2+78.158Z-316.03, \quad (44)$$

(Elements 11-18);

$$E_{e-e}(\text{in atom})=-0.1548z^3+17.055z^2-394.45z+3159.7, \quad (45)$$

(elements 25-29).

The difference between eq. (46) and eqs. (47)-(50) is eq. (43). The significance to establish eqs. (43)-(45) is found and verified electronic configuration rules in atom from them. The accuracy of the correlation coefficient of the mapping tool is not enough, the merits of the regression equation can not be judged according to them. We have to use this stupid way of calculation of relative error to choose the best regression equation.

Take fluorine atom as an example, substituting $z=9$ into eq. (47), we can obtain

$$-E(F)^{(0)}=45489.6+300915-100296+18178=264286.6 \quad (\text{KJ/mol}).$$

The experimental value is $E(F)^{(0)}=-262040.5$ KJ/mol. The relative error is 0.9%. Substituting $Z=9$ into Eq. (48), we can obtain

$$-E(F)^{(0)}=45416.7+301311.9-101034+18572=264266.6 \quad (\text{KJ/mol}).$$

The relative error is 0.9%.

Substituting $Z=9$ into Eq. (49), we can obtain $-E(F)^{(0)}=45854.1+298533.6-95733+15552=264206.7$ (KJ/mol). The relative error is 0.8%. Substituting $Z=9$ into Eq. (50), we can obtain

$$-E(F)^{(0)}=36012.6+339106.5-147951+35457=262624.6 \quad (\text{KJ/mol}).$$

The relative error is 0.2%. The greater the atomic number, the greater the error of the ionization energy, so, the more points to be involved, the worse the effect to fit. The quantum mechanical calculation method above can be called the regression equation method (or fitting curve method).

Regression equation perturbation method or fitting perturbation method: improvement of the traditional perturbation method

If somebody obsessed with the traditional perturbation method, we also have a way. The method is to combine the regression equation with the perturbation method. The principle is: the known term of interaction energy between electrons in the system was greatly increased in regression analysis, the energy of the unknown term is greatly reduced, at this point, the results to use perturbation method is better than the one of traditional method.

Way one: Assuming there is a smaller error using Eqs. (47)-(50) to calculate the energy of the atom. Eqs. (47)-(50) can be boiled down to a potential energy function, the error can be boiled down to a perturbation term, and then calculate.

Way two: The potential energy functions are divided into three categories: the first category is the potential energy of pure electrons; the second category is the interaction potential energy between electrons known by the method in this paper; the third category is a perturbation term. Take Oxygen atom as an example.

$$E(O)^{(0)}=[2E_{n-e}(1s^1)+2E_{n-e}(2s^1)+4E_{n-e}(2p^1)]+[E_{e-e}(1s^2)+E_{e-e}(2s^2)+2E_{e-e}(1s^2-2s^1)+5E_{e-e}(2p^{\uparrow\uparrow})+4E_{e-e}(1s^2-2p^1)+4E_{e-e}(2s^2-2p^1)]+E_{e-e}(2p^{\uparrow\downarrow}) \quad (51)$$

The first part is expressed by using a few $-aZe^2/r$ (notice the difference in the main quantum number and the coefficient of the difference). The second part is expressed by using bZ^*e^2/r_{ab} . Do not need to make a concrete form.

The third part of the potential energy function can be written in the form of $\lambda e^2/r$. This part is the sum of the

relativistic effect, the volume effect and the penetration effect. Relative to the total energy, the $\lambda e^2/r$ is very small.

Table 4: The relationship between “energy of some atoms and atomic cores” and the atomic numbers.²

Elements	Z	$\Sigma Z^2/n^2$	$\Sigma I(\text{atom})$	$\Sigma I(\text{C-like ion})$	$\Sigma I(\text{N-like ion})$	$\Sigma I(\text{Ne-like ion})$	$\Sigma Z^2/n^2 - \Sigma I$
Li	3	26583.3	19633.3				6950.0
Be	4	52510.2	38511.9				13998.3
B	5	90251.8	64739.9				25511.9
C	6	141777.4	99390.3	99390.3			42387.1
N	7	209056.1	143382.9	141980.6	143382.9		65673.2
O	8	294056.9	197195.9	192493.7	195882.0		96861.0
F	9	398749.0	262040.5	250934.9	256985.3		136708.5
Ne	10	525101.6	338821.0	317295.0	326666.0	338821.0	186280.6
Na	11	653022.2	426461.1	391596.0	404950.0	425965.3	226561.1
Mg	12	798154.4	525952.6	473839.0	491859.0	523764.2	272201.8
Al	13	961374	637383	564120	587446	632244	323990
Si	14	1143555	761101	662187	691474	751150	382454
P	15	1345573	897876	768331	804236	880806	447697
S	16	1568303	1047791	882502	925679	1021126	520512
Cl	17	1812622	1211346	1004672	1055731	1171905	601301
Ar	18	2079412	1381933	1134837	1194480	1292678	697498
K	19	2346485	1580397	1273033	1341983	1505813	766088
Ca	20	2632802	1785893	1419533	1498423	1689053	846909
Sc	21	2966988	2005570	1573963	1663453	1882943	961402
Ti	22	3326428	2240432	1736554	1837254	2087429	1086434
V	23	3713363	2491224	1907334	2020034	2302954	1222119
Cr	24	4127302	2731814	2086393	2211693	2529303	1395463
M	25	4569569	3040968	2273497	2412097	2766777	1528601
Fe	26	5041048	3318898	2466861	2619461	3013161	1722123
Co	27	5542611	3658305	2672893	2840293	3274972	1884277
Ni	28	6075133	3992411	2884876	3067576	3544676	2082691
Cu	29	6639492	4345619	3105423	3304223	3826923	2293836

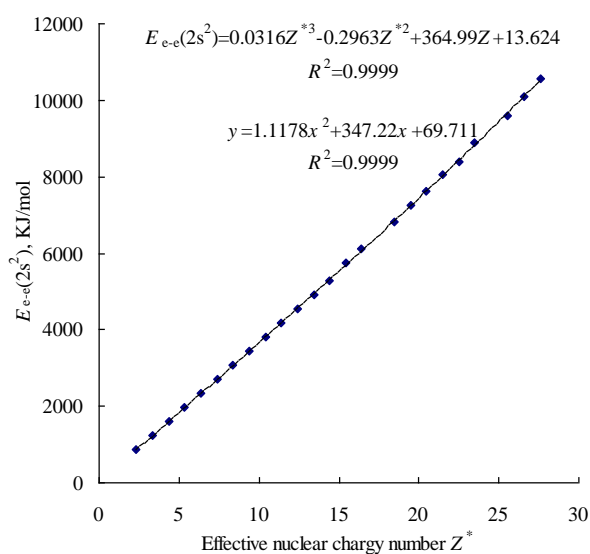


Figure S1: Effective nuclear number

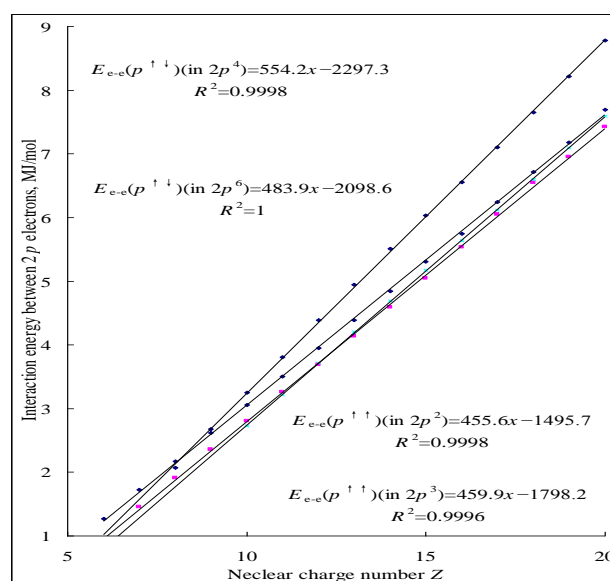


Figure S2: Nuclear charge number.

DISCUSSION

The significance of the relationship between the ionization energy and the interaction energy of elements

The research results presented in this paper have three highlights: (a) some new rules about ionization energy of elements have been found, the relationship between “the interaction energy of electron-electron, atomic energy” and the nuclear charge number have been summed up; (b) the experimental principle of measuring the interaction energy of electrons is established; (c) the method of fitting quantum mechanics is invented. These highlights have enlarged human knowledge.

The results of this paper not only can increase the human knowledge, but also have a wide range of applications. Accurately calculating the energy of a complex atom with a simple method is the dream of mankind. But, in the last hundred years, this dream has not been realized. In this paper, we have achieved this dream. Eqs. (47)-(50) and the regression equation for calculating the energy of the atom core can make the ab initio calculation in quantum chemical method of ab initio calculation is no longer required. The combination of regression equation method (fitting method) and perturbation method can make the subjective factors in the traditional perturbation method greatly reduced. Since we can calculate the interaction energy between electrons in the atom, can calculate the average distance between electrons. The experimental principle and method of measuring the interaction energy between electrons is also the principle and method of measuring the average distance between electrons.

Need to do the work as following: Measure out more accurate and more ionization energy values; fit out more regression equations of atom-like ions (In the 107 elements, at least 100 of the regression equations of the atom cores need to be fitted); List complete regression equation of the atom core for researchers to use; Study on, after the outer electron ionization, the influence of inner electron rearrangement upon the measurement of atomic energy.

In addition, we'd better extend the theory and methods of these principles to the calculation of the molecules.³⁻⁵ We can Measure the free electron pairing energy. Use of the analysis for the ionization data, we can further study on the electronic arrangement. We can use the same principle and method to find the interaction regularities between electrons in *d* sub layer and *f* sub layer. We can establish the concept of "average distance between electrons".

In the past, quantum mechanical calculations involving the interaction between electrons are all approximate calculations. This severely limits the application of quantum mechanics. Although the calculation of complex system with quantum mechanics is very complicated and the accuracy is too low, quantum mechanics is still widely used in the fields of atomic physics, chemistry,

and physics and so on. Now, the interaction between electrons can be more accurately calculated. The application effect of quantum mechanics will be better, and the application scope will be further expanded. The some places have not applied the quantum mechanical calculation because of the calculation to be complexity and accuracy low, and now can be applied.

Literature classification of this paper: A cross discipline of quantum chemistry and quantum mechanics, and belong to the basic research in the application of quantum mechanics. In this regard, human beings have not been a major breakthrough in many years. This is also an important factor which gives rise to the interest of more scientists.

Mendeleev found that the periodic law of elements is only found that the nature of the element with the atomic weight of periodic changes, the use of the technology is inductive method. Planck was only based on the formula of existing black body radiation in the long wave range applicable and the formula in the short wave range applicable to get an interpolation formula. The technique he uses is a deductive method. My work is to get the relationship between the interaction energy of the electron and the atomic energy and the nuclear charge number. I also use the inductive method. The relationships I've had before are not, and should belong to the original work. If you say that my work is not high technical content is not innovative, then, both Planck and Mendeleev's works are not innovative, nor the research results of high technical content. If only the work of Mendeleev and Planck were to be recognized, the originality of my work would not be recognized. This is prejudice.

I think that, high technology content is not the most important; the most important is the application of value. It is undeniable that the work of this paper can be applied to all occasions that need to calculate atomic and molecular energy. It can greatly reduce the workload of researchers who need these calculations. Originally, these regression equations that can be used to calculate atomic energy based on the number of nuclear charges did not appear in the world, and in this paper appeared, they are the author's original creation. If you do not think this is the original, that is, the use of a double standard. Who knows the atomic energy of element 107? I know.

For the calculation of the complex atomic system, it is undoubtedly a scientific progress to create a quantum mechanical method without trial function.

Few references are likely to be similar to previous studies. Einstein wrote the first article on the theory of relativity there is no reference. According to the author's background and the use of the reference literature to assess the level of the article, for others may be basically the right. But, for my article can only be wrong and unjust.

Funding: No funding sources

Conflict of interest: None declared

Ethical approval: Not required

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Cite this article as: Tu R. The principle and application of experimental method for measuring the interaction energy between electrons in atom. *Int J Sci Rep* 2016;2(8):187-200.