MODELING OF THE SPATIAL STRUCTURE OF THE ATOM.
PART I. ELECTRONIC SHELL

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Summary
This paper presents an approach that allows describing the spatial formation of the electron shells of atoms, based on known principles and rules, in a logically consistent version of the visual representation of an atom. The proposed model makes it possible to estimate the location of electrons in the electron shell visually, as well as to determine the quantum numbers responsible for the position of electron clouds in an atom. We have developed computer models of real atomic structures based on known experimental and calculated data on orbital radii and ionization energies.

Key words: computer modelling; electron shell; atom; ionization energy; shell model; quantum number; electron cloud.

1. INTRODUCTION

The basis of modern concepts of science is the fundamental idea according to which any properties of objects of the surrounding world can theoretically be deduced from the characteristics describing the structure of material objects through the construction of models [1]. One of the tasks of the physical orientation is the modeling of the electron shell of an atom in order to visualize the distribution of electrons inside the atom. To date, a sufficiently large number of models of atoms have been proposed [2]. With all the variety of models of the electronic structure of atoms, the most famous of them is the shell model [3]. The shell model of a multi-electron atom is based on the hypothesis of the separation of electrons into certain groups, called electron shells. The electron shell is usually understood as a set of electronic orbitals, which are characterized by four quantum numbers: *n – the main one; l – orbital;* m_l *– magnetic and* m_s *– spin quantum number* [4].

The rules for filling atomic orbitals in a multielectron atom are based on three main principles [5]: the lowest energy, the Pauli exclusion principle, and the highest multiplicity for the ground states of the electron shells of atoms (Hund's rule). According to the principle of minimum energy, the most stable state of an atom corresponds to the placement of electrons in orbitals with the lowest energy, i.e. the minimum potential energy of a system consisting of a set of electrons and a nucleus is provided. Also important in the atom is the Pauli principle, which prohibits the presence of more than one electron with the same set of four quantum numbers (n, l, m_l and m_s). If all states are occupied for the principal quantum number with a certain value, then it is customary to speak of the formation of a closed (closed) shell. The principle of maximum multiplicity allows the population of orbitals by electrons within a separate subshell in such a way that the modulus of the sum of spin numbers is maximum [7]. The order of increase in atomic orbital energies in multielectron atoms is described by the Klechkowski rule [8]: with an increase in the charge of the nucleus of an atom, the filling of orbitals occurs in the order of increasing sum of the main and orbital quantum numbers ($n+l$), and with equal values of this sum, in the order of increasing n.

To visualize the distribution of electrons in atoms, it is customary to use several different methods, the main of which are analytical notation and the quantum cell method [6]. An analytical notation is an alphanumeric electronic formula, which is built from *nl*-subshells with an indication of the number of electrons that populate each of them. Guided by the principles of minimum energy and Pauli, as well as the rules of Hund and Klechkowski, one can determine not only the order in which orbitals are populated by electrons, but also construct the electronic formula of any atom. The disadvantage of alphanumeric electronic formulas is the use of only two quantum numbers n and l.

An electronic circuit is a symbolic model that does not represent a three-dimensional image of the electronic shell. It is intended only to reflect the sequence in which each electron shell is filled. When studying the properties of atoms, it is possible to simulate the structure using the quantum cell recording method. The cells included in the cell scheme can be populated with electrons. Each specific variant of settlement is called the electronic configuration of the atom. According to the values of quantum numbers *n* and *l* the cell scheme can be divided into *n-shells* and *nl-subshells*. Based on the recording of electronic configurations by subshells, this method takes into account the maximum number of quantum cells of the electron subshell, into which electrons are populated. We should also note that not only the electronic configurations of an individual selected subshell with completely filled, but also half-filled orbitals are characterized by increased stability.

Modern ideas about the structure of the atom electron shell come from the fact that the motion of an electron in an atom cannot be described by a certain trajectory. It is possible to consider only a certain volume of space in which the electron is located, which is called the electron cloud [9]. The electron cloud is a visual model that reflects the distribution of the probability density function of finding an electron in an atom depending on its energy. At the same time, if we have a certain maximum probability at a certain point of the electron cloud, then taking it as the center of the cloud and assuming that the electron itself is located at this point, we can estimate the size of not only the cloud, but also the atom itself.

In the geometric model [10], the size of the spheres denoting electron clouds depends on the charge of the nucleus and the proximity of the shell to the atomic nucleus. The geometric model combines the advantages of both electronic circuits and orbital models. In addition to the above, the geometric model also has a number of new features: demonstrating the stability of certain electron shells in an atom, assessing the location of electrons in an atom, and also allows you to deal with atomic numbers 2, 10, 18, 36, 54, 86, 118, which are a common the number of electrons in the inner filled electron shells.

At the beginning of the 20th century, A. Parson [11] suggested that electrons do not revolve around the nucleus, but under the influence of electromagnetic field forces, at a certain finite distance from the nucleus, they come into stable equilibrium with electrons located in spherically symmetric stable configurations. At the same time, in his model, electrons are located at stationary positions around the nucleus. In developing this hypothesis, J. Langmuir proposed to take into account a number of other structural features of the atom [12]:

1. Electrons in atoms are located in paired planes symmetrical with respect to the nucleus. Atoms have an axis of symmetry perpendicular to these planes.
2. Each cylindrical layer breaks up into several cells of equal volume.
3. Electrons act on each other with mutually balanced electrostatic and electromagnetic forces.

In the future, in the theory of M. Gryzinsky [13], which is based on the ideas of A. Parson and J. Langmuir, it was confirmed that the electrons in the atom are arranged regularly, the atom itself has an axis of symmetry and, most importantly, the electrons move collectively, due to the presence of a periodic component in the electric field of the atom. Moreover, he came to the conclusion that atoms can be described by classical Newton's equations using known interactions without introducing free parameters. Additionally, we note that the structure of the atom, despite the presence of a number of models, has not yet been fully deciphered. However, we will assume that it can be reproduced in graphical form on the basis of already known experimental and theoretical data. It is for this reason that the main task set in this paper is to visualize the physical representation of the spatial structure of the electron shell of an atom by computer modeling it as a collection of electron clouds located near the nucleus of an atom.

2. SIMULATION

Our main task is to understand how the electron shells of an atom are housed, and how the spatial structure changes as it becomes more complex. The main object of simulation in our study will be an isolated atom in a normal state. In an atom, the system under study is a collection of electrons located in the Coulomb field of the nucleus. Let's assume that we can mentally dive into the atom and visually control the position of the electrons. At the same time, the explanation of the behavior of any individual electron in the composition of an atom is possible only on the basis of knowledge of its general properties, described using a set of known principles and rules.

To solve the problem set before us, the most useful is the shell model of a multielectron atom. As a basis for constructing the electron shell, we take the well-known principles: the minimum of potential energy, symmetry and the Pauli principle. The principle of minimum energy is basic in constructing the electronic configuration of an atom, since the presence of a certain amount of electron energy is a consequence of the electron being on the corresponding shell of the atom.

Within the framework of this approach, we will assume that the electron is a structureless material point located in the center of its own electron cloud, and the position of the electron in the near-nuclear space can be set by a set of quantum numbers. For a detailed disclosure of the structural properties of the electron shell of an atom, we will need to visualize the internal structure of the atom by computer modeling based on known experimental data on the location of electron clouds around the atomic nucleus without using a quantum mechanical approach.

Suppose an atom has several components, the most important of which in our study can be considered dynamic and static. In accordance with the formulation of the problem, the dynamic component is rigidly connected to the nucleus of an atom, considering its behavior as an object connected into a single whole with electron clouds. When accepting the hypothesis of the rotation of the atom as a whole [13] and, consequently, the use of a static representation of the atom allow us to exclude from our consideration such dynamic concepts as orbital and spin quantum number. This approach will also make it possible not to consider the influence of relativistic effects.

Initially, we turn to the definition of a method for modeling the electron shell of an atom. To do this, we will choose a cylindrical coordinate system, in the center of which we will place the nucleus of the atom (Fig. 1).

One of the axes, for example, the polar axis *Ox*, will be selected as the base, relative to which the rotation of the entire atom as a whole will occur. Given that the x coordinate must be included in the set of quantities responsible for the positions of the electron clouds in the atom, we assign it the name of the basic quantum number.

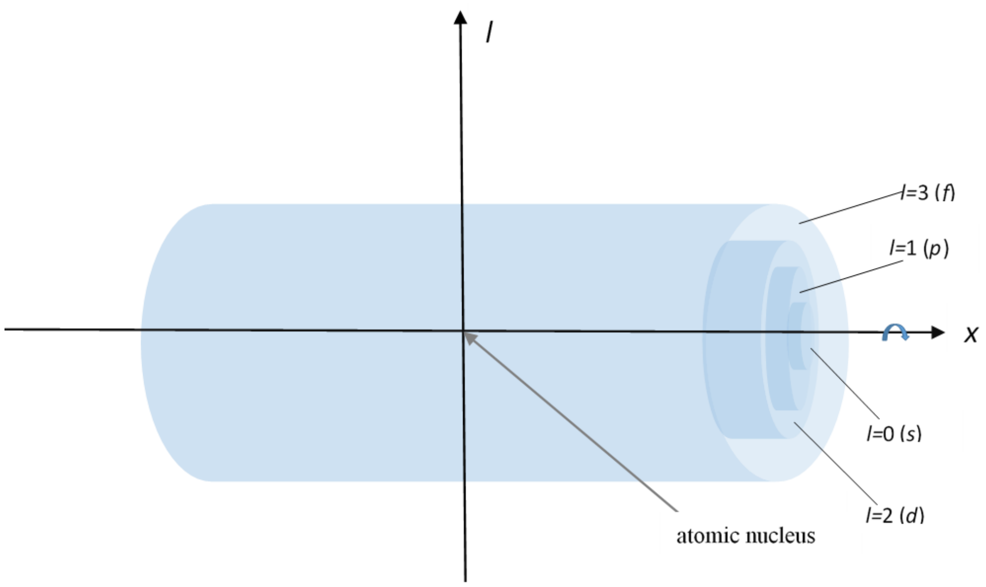


Fig. 1 Schematic view of the atom electron shell

In this case , the choice of the value of the main quantum number *n* will be calculated by the formula

$$n = mod(x) + l\,, where\ x \neq 0\,. \tag{1}$$

In this case, the principal quantum number determines only the number of the electron shell and will not be used in estimating the positions of the electrons. The applicate axis *Oz* is compatible with the orbital quantum number *l*. By choosing certain values for the quantum numbers *x* and *l* one can unambiguously find out on which of the electron shells the electron is located, with which these quantum numbers are associated. The role of the third coordinate here is played by the azimuthal angle, positioned as the angle of rotation around the polar axis *Ox* and characterized by the magnetic quantum number m_l. The magnetic quantum number determines the possible orientations of electron clouds in space. The number of such orientations is known to be: $2l+1$. Based on the change in the set of quantum numbers, it is also necessary to modify the Pauli principle, which can be limited to the use of three quantum numbers: basic, orbital and magnetic to determine the spatial arrangement of the positions of electron clouds.

In this work, the shell model of an atom is taken as the starting point for creating a computer model of the electron shell of an atom, remaining within the framework of classical electrostatics. For our consideration, the principle of indistinguishability of electrons is also important, according to which all electrons of a separate shell are equal in rights and are equally connected with the nucleus [14]. The shell model is supplemented by the assumption of a symmetrical configuration of electrons in each of the shells, which satisfies the condition of minimum potential energy and ensures the stability of the atom.

When choosing the objects that make up the electron shell of an atom, it is necessary to take the electron clouds formed by them as a basis as visual objects instead of the electrons themselves. Suppose we have a collection of electrons near the nucleus of an atom in a normal state, each of which forms its own electron cloud around itself. For the purpose of simplification, we will consider only spherical electronic clouds located on the corresponding shells and subshells. When determining the location of clouds, we will assume that the area of their placement is some area of space not surrounding, but located near the nucleus of an atom.

Each electronic cloud is characterized by the following main parameters:

– nuclear charge: it is assumed that the charge is concentrated in the center of the electron cloud;

– the radius of the electron cloud of finite size;

– spatial coordinates determined on the basis of quantum numbers.

For convenience of representation, taking into account the selected value of the orbital quantum number, each of the electron clouds can be associated with certain color designations (Table 1).

Table 1. Color identification of electron clouds, according to the values of the orbital quantum number

Orbital quantum number	*s*	*p*	*d*	*f*
Colour	Yellow	Green	Red	Blue

To fix the static nature of the structure, we assume that there are no processes of reconfiguration of electron clouds near the nucleus in this model, except for the settlement of subshells by kainosymmetries. It does not provide for taking into account the mechanical inertia of particles, determined by their mass, as well as taking into account their own rotational motion of particles. We will also assume that all kinetic energy is concentrated only in the rotational motion of the entire atom as a single whole.

To fix the static nature of the structure, we will assume that there are no reconfiguration processes of electron clouds near the core in this model, except for the colonization of subshells by kainosymmetrics. There is no provision for taking into account the mechanical inertia of particles determined by their mass, as well as taking into account their own rotational motion of particles. We will also assume that all kinetic energy is concentrated only in the rotational motion of the entire atom as a whole.

Summarizing all the explanations considered, it was decided, when conducting computer modeling of the spatial structure of the electron shell of an atom, to accept the following assumptions:

1. Only atoms in a normal state are considered.

2. Electron clouds have a spherical shape and a finite radius. Each electron cloud occupies a certain area near the core and does not intersect with neighboring clouds or the core itself.

3. The atom as a whole is in a state of rotation around some selected basic axis.

4. The modified Pauli principle determines the spatial arrangement of electron clouds relative to each other and relative to the nucleus of an atom, and is based only on three quantum numbers: x, l, and m_l.

5. The magnetic quantum number ml makes it possible to determine the number of electrons placed on a common plane perpendicular to the base axis at a given value of the orbital quantum number l.

6. The principle of minimum energy determines the order of settlement of electrons having different values of potential energy.

7. The interaction of electrons with each other and with the nucleus is calculated in accordance with Coulomb's law, and the resulting interaction is determined by the sum of its interactions with all others.

8. The settlement of electrons in a multi-electron atom, in the main, that is, the most energetically advantageous state, occurs in accordance with previously established principles and rules.

9. The model does not take into account the finite mass of the nucleus, its size and relativistic effects.

To verify the basic provisions of the model of the formation of the spatial structure of the atom electron shell, a software package was created in which an electrostatic mechanism of interaction of electrons with each other and with the nucleus of an atom was implemented. In order to obtain a structure similar to a real atom, the orbital radii of each electron were taken into account [15], and the location of the electron clouds was determined based on known data on ionization energy [16], and for s-electrons by additional calculation of their radii for all values of the main quantum number.

3. RESULTS AND DISCUSSION

3.1 SIMPLE MODEL

Let us assume that the electron clouds that make up the electron shell of the atom are objects that have equal unit diameters. Let us mark the *Ox* axis (Fig. 1) in units numerically equal to the diameter of the electron cloud (hereinafter, instead of the concept of "electron cloud" we will use the concept of "electron", however, if it becomes necessary to note their difference, we will indicate them separately). We will demonstrate the operation of known principles and rules using specific examples.

Atomic number *Z*=2. The first shell, which has the smallest capacity, is represented by two atoms with charge numbers $Z = 1$ and $Z = 2$ (Fig. 2). In an atom with $Z = 1$ there is only one electron, whose position is determined by quantum numbers: $x = 1$, $l = 0$, $m_l = 0$, which will occupy the 1*s*-оболочку shell and in the ground state will have an electronic configuration of $1s^1$.

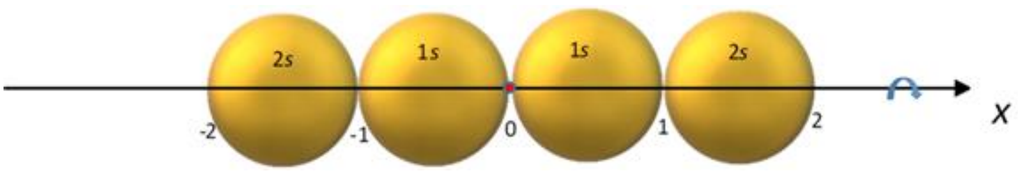


Fig. 2 Example of the arrangement of electron clouds in an atom

The second electrons, in accordance with the principle of minimum energy, will also occupy the 1*s*-shell and the atom in the ground state, in turn, will have a completed electronic configuration of $1s^2$. But in order to comply with the modified Pauli principle, this electron must have a difference from the first in its set of quantum numbers (x,l,m_l). The only quantum number that can be changed "to enter" this shell is the base quantum number. Thus, on the 1*s-shell*, in addition to the first electron with a set of quantum numbers (1,0,0), there will also be a second electron with a set (-1,0,0). Therefore, in accordance with these principles, both 1*s* electrons will complete the occupation of the K-shell.

Atomic number *Z*=4. In an atom with $Z = 3$ the first two electrons are already fixed on the 1*s*-shell, therefore, by virtue of the Pauli principle, the third electron cannot be attached to the first two. It falls on the next 2*s*-subshell (Fig. 2), i.e. with a set of quantum numbers (2,0,0). The fourth electron will occupy the same 2*s*-subshell having a similar set of quantum numbers, differing only in the value of the base quantum number (-2,0,0). Now the 2*s*-subshell will also be completely filled, while the atom will already have an electronic configuration – $1s^2 2s^2$.

Atomic number *Z*=10. Due to the fact that the capacity of the 2*s*-subshell is also limited to two electrons, the next atom with an atomic number Z = 5 occupies the 2*p*-subshell, having a set of quantum numbers (0,1,1) (Fig. 3).

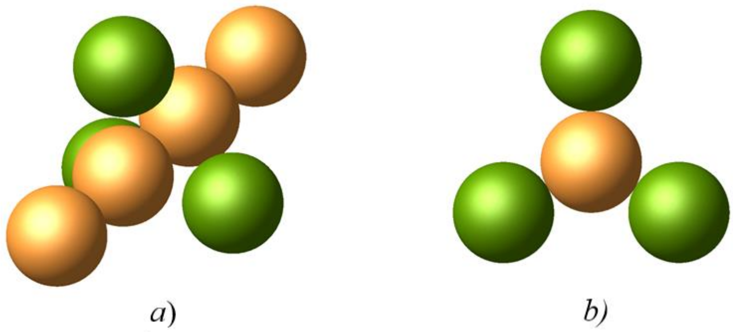


Fig. 3 Model of electron shells for $Z = 7$ in two projections:
a) in a plane passing through the axis of rotation of the atom at an angle of 45^0;
b) in a plane perpendicular to the axis of rotation and passing through the center of the core.
– *s*-electrons, – *p*-electrons

All 2*p*-electrons are usually referred to as kainosymmetrics. An atom with a charge number Z = 6 will be arranged symmetrically and will have a set of quantum numbers (0,1, -1).

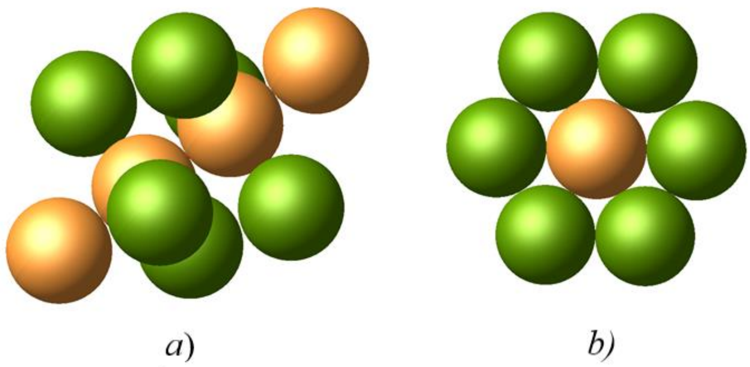


Fig. 4 A simple model of electron shells for the first 10 electrons in two projections:
a) in a plane passing through the axis of rotation of the atom at an angle of 45^0;
b) in a plane perpendicular to the axis of rotation and passing through the center of the nucleus.
– *s*-electrons, – *p*-electrons

Further occupation of electrons, starting from Z = 7 with a set of quantum numbers (0,1,0), will already lead to a transformation of the spatial arrangement of 2*p*-electrons. All three of the first 2*p*-electrons (from the fifth to the seventh) will be located symmetrically relative to the axis of rotation of the atom and each other. Here, the well-known Hund’s rule is automatically fulfilled when all three 2*p*-electrons have the same value of the base quantum number. The remaining three electrons, from the eighth to the tenth, are populated to their positions with the base quantum numbers x = -2 while simultaneously shifting the previously set 2*p*-electrons, changing the values of the base quantum number for all previously occupied 2*p*-electrons to the value – x = *2*. At this stage, the filling of the *L*-shell of the atom is completed (Fig. 4).

Atomic number *Z*=18. The next closed stable configuration of electrons is formed by occupying the 3*s*- and 3*p*-subshells that make up the *M*-shell of the atom with electrons. These include atoms with Z = 11 to Z = 18 (Fig. 5). Note that, starting with the consideration of the charge number Z = 11, we will refrain from specifying specific sets of quantum numbers for individual electrons.

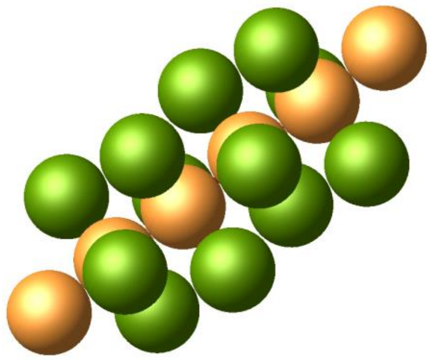
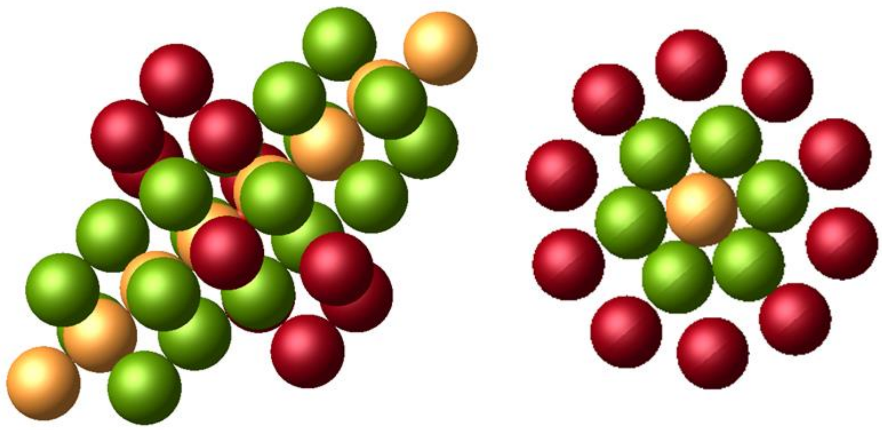


Fig. 5 A simple model of the electron configuration with the charge number of the atom Z = 18.
– *s*-electrons, – *p*-electrons

When analyzing the positions of the electrons in this configuration, it can be seen that the principle of minimum energy should indicate the initial occupation of 3*p*-electrons. However, in a real atom, there is a significant compression of 1*s*-electrons, as well as some compression of 2*s*-electrons, leading to a change in the ratio of the positions of the electrons relative to the nucleus of the atom. For the same reason, in the future, 4*s*-electrons will also occupy earlier than 3*d*-electrons.

Atomic number *Z*=36. Filling the electron shells to form an atom with Z = 36 leads to the occupation of 4*s*-, 3*d*- and 4*p*-subshells. These include atoms from Z = 19 to Z = 36 (Fig. 6).



a) *b*)

Fig. 6 A simple model of the configuration of electrons with the charge number of the atom Z = 36:
a) in a plane passing through the axis of rotation of the atom at an angle of 45^0;
b) in a plane perpendicular to the axis of rotation and passing through the center of the nucleus.
– *s*-electrons, – *p*-electrons, – *d*-electrons

At first, as noted above, there is an occupation of the *4s*-subshell. After filling it, the occupation of the *3d* subshell begins, the capacity of which is 10 electrons. In the six subsequent atoms from Z = 31 to Z = 36, the electrons are already located in the *4p* condition.

Atomic number *Z*=54. The presented group of atoms is similar in structure to the previous one (Fig. 7). Both groups have the same capacity and contain 18 atoms each. Here, at first, there is an occupation of the 5*s*-subshell. After its filling, the occupation of the 4*d-sub*shell begins, and the formation of the electronic configuration is completed by the occupation of the 5*p-sub*shell (Fig. 8).

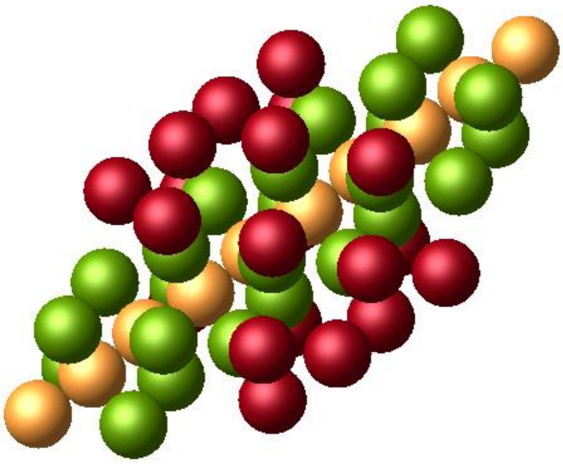


Fig. 7 A simple model of the electron configuration with the charge number of the atom Z = 54.
– *s*-electrons, – *p*-electrons, – *d*-electrons

Upon further consideration, we will no longer take into account the natural order of electron occupation, which is determined by the principle of minimum energy and has a number of deviations in the order of occupation of the atom shells.

Atomic number *Z*=86. This is followed by one of the most representative groups of atoms, containing 32 different configurations (Fig. 8). In these atoms, respectively, the 6*s*-, 4*f* - and 5*d*-subshells are occupied with electrons. The occupation of free positions with electrons is completed by filling the 6*p*-subshell.

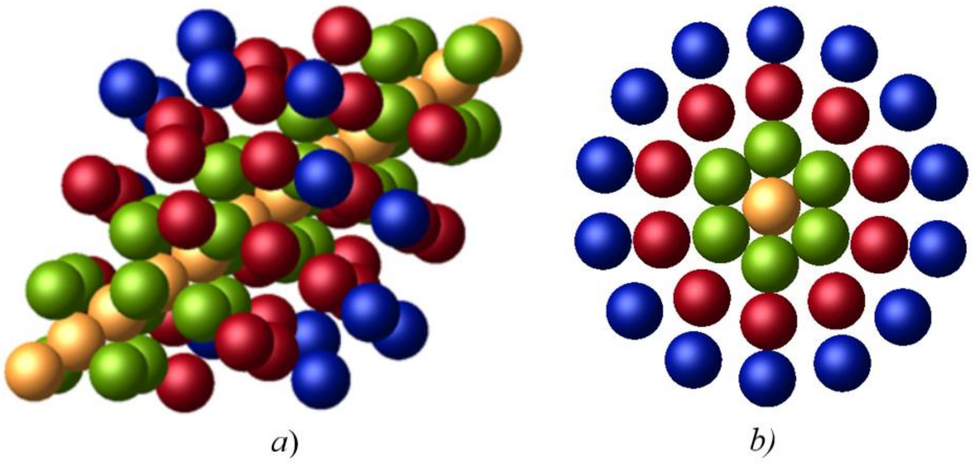


Fig. 8 Simple model of electron configuration with atom charge number Z = 86:
a) in a plane passing through the axis of rotation of the atom at an angle of 45^0;
b) in a plane perpendicular to the axis of rotation and passing through the center of the core.
– *s*-electrons, – *p*-electrons, – *d*-electrons, – *f-electron*s

Atomic number *Z*=102. Similarly, the occupation of subshells occurs in heavy atoms. However, due to the presence of an upper bound of the atomic number, with the parameters of atoms available for analysis, we will limit ourselves only to the population of 7*s*- and 5*f*-subshells with electrons (Fig. 9). The capacity of these subshells will be equal to 16 electrons.

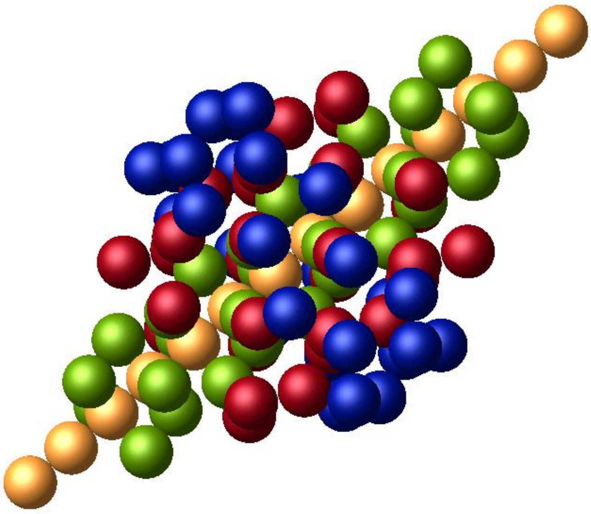


Fig. 9 A simple model of the electron configuration with the charge number of the atom Z = 102. – *s*-electrons, – *p*-electrons, – *d*-electrons, – *f*-electrons

When considering the electronic configuration of an atom with Z = 102 we pay attention to a certain elongation of *s*-electrons along the polar axis, resulting from the absence of *ns*-electrons in a simple compression model.

At the end of the consideration of a simple model of electron shells, we will check for compliance with the dependence of the first ionization energy E_i on the charge number Z for light atoms (Fig. 10).

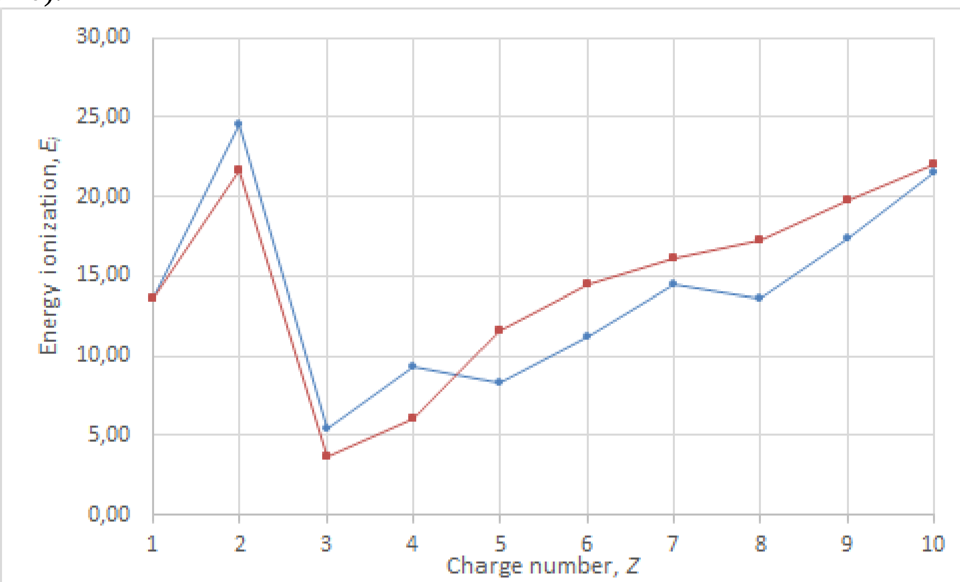


Fig. 10 Dependence of the first ionization energy E_i on the charge number Z: – empirical data [16], – simple model

Calculations of ionization energies were carried out without taking into account the dynamics of electron displacement during the formation of the electron shell for all *K*- and *L*-shell atoms. As can be seen on the graph, the trends of ionization energy changes for the values of the first ionization energy E_i of model atoms and empirically obtained data have a common direction, which indicates a certain correspondence, even within a simple model, to the real nature of the behavior of this parameter of the electron shell of an atom.

3.2 DIMENSIONAL MODEL

The actual sizes of the electron clouds that make up the spatial model of an atom differ, depending on their position relative to the nucleus. Their size qualitatively reflects the magnitude of the binding energy of electrons on individual subshells. The greater the binding energy of the electron to the nucleus in the subshell, the smaller the size of the sphere modeling the electron cloud should be. Therefore, by the dimensional model of the electron shell of an atom we will understand a set of electron clouds, each of which has an electron in its center located at a distance of its orbital radius from the nucleus. The principal advantage of the proposed method of visual representation of the atom is that the data of empirical measurements and calculated values of the parameters of the atom are jointly used here to visualize the electronic shells of atoms, and not, as is generally accepted, to determine the parameters of atoms. This approach allows us to take a different look at the possibilities of studying and predicting the properties of multielectron atoms.

When forming the spatial structure of the electron shell of a dimensional model of an atom, we will take as a basis, when determining the positions of electrons, such parameters of the atom as the distances between the nucleus and individual electrons (orbital radii), the distances between the electrons themselves, as well as the first ionization energies of atoms.

The occupation of *s*-electrons will be carried out taking into account the empirical and calculated values of the orbital radii. At the same time, to determine the size of *s*-electrons, we will choose the radius of the electron cloud R_s, obtained by calculating for the values of the main quantum number $n > 1$ for the corresponding orbital radii $r_{\text{орб}}$ according to the formula

$$R_s(n) = r_{\text{орб}_n} - 2\sum_{i=1}^{n-1}(-1)^{i+1}\, r_{\text{орб}_i}\,. \tag{2}$$

At the magnitude of the main quantum number $n = 1$ the radius of the electron cloud is identical to the minimum orbital radius: $R_s(1) = r_{\text{орб}_1}$. The values of the orbital radii are taken from the previously performed work [15].

When occupying *p*-, *d*- and *f*-electrons, it is necessary to use an additional parameter, defined as the interval ΔR between symmetrically arranged positive and negative electrons in the base quantum number belonging to the same subshell (Fig. 11). Note that the diameters of the electron clouds of all shells, with the exception of the *s*-shell, in order to increase the clarity of the representation of the electron shell of the atom, are shown in the figure in a halved size.

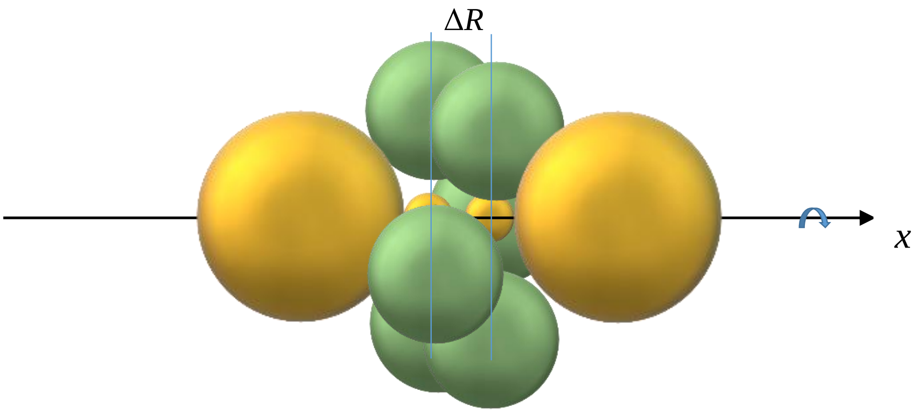


Fig. 11 The interval ΔR between the 2*p*-electrons of the semi-closed parts of the subshell

To estimate it a priori, we assume that it is proportional to the size of the corresponding orbital radius

$$\Delta R = 2Ar_{\text{орб}}\,, \tag{3}$$

where A – is the proportionality coefficient that determines the amount of electron displacement relative to the polar plane; $r_{\text{орб}}$ – is the radius of the electron cloud. A multiplier numerically equal to two is included in the formula to account for the size of the entire value of the interval ΔR between the centers of electrons symmetrically located semi-closed parts of the subshell.

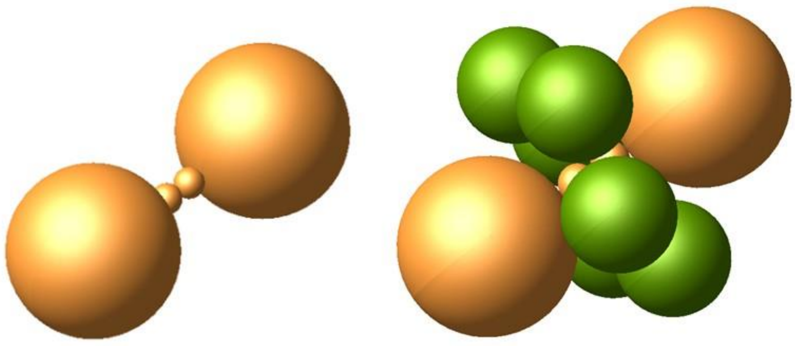
For example, the 2*p*-electrons, positive in the base quantum number, are located in parallel symmetrical planes with respect to having a negative base quantum number, relative to the plane passing through the center, perpendicular to the horizontally located main plane. Empirical data on the ionization energy can be used to determine the ΔR interval [16]. By shifting these symmetrical planes along the polar axis *Ox* (Fig. 11), we achieve a coincidence of the calculated and empirical values of the ionization energy for the electron shell of the atom under consideration. So, for a 2*p*-subshell, the first ionization energy of an electron is $E_i\,(Z=10)$ = 21.5645 MeV. The selection of the interval at which the calculated ionization energy will also have a similar value leads to the value: $\Delta R = 0.24 r_{\text{орб}}$ (Fig. 11). Using the obtained values of the interval, it is possible to carry out the settlement of 2*p*-electrons with negative base quantum numbers (Fig. 13). The selection of the values of the coefficient *A* for the interval ΔR was carried out once for each subshell and was fixed for all other atoms (Table 2).

Table 2. Values of coefficient *A* for the interval ΔR
between the semi-closed parts of individual subshells

Subshell's name	Atomic number, *Z*	Ionization energy, E_i (M*eV*)	Coefficient *A*
2*p*	10	21.5645	0.1193
3*p*	18	15.7596	0.8772
3*d*	30	9.3942	0.9091
4*p*	36	13.9996	0.8214
4*d*	46	8.3369	0.8460
5*p*	54	12.1298	0.7800
4*f*	70	6.2542	0.7666
5*d*	80	10.4375	0.8525
6*p*	86	10.7485	0.7564
5*f*	102	6.6600	0.7767

Let us now turn to the consideration of specific dimensional models of atoms having only closed subshells.

Atomic number *Z*=2, *Z*=4 and *Z*=10. 1*s*- and 2*s*-subshell are populated by electrons similarly to their representation in a simple model. However, in the process of increasing the atomic number of the nucleus, the size of the electron clouds of 1*s*-electrons decreases significantly, and 2*s*-electrons visually dominate them (Fig. 12a). The large size of the 2*s*-subshell electron clouds also affects a significant decrease in their ionization energy.



a) *b)*

Fig. 12 Dimensional models for closed electron shells of an atom:
a) $Z = 4$; *b)* $Z = 10$

Let's pay attention to the size of the electron clouds of the *p*-shell, as well as the size of the electrons of other shells (with the exception of s-electrons). Considering that the actual sizes of these electron clouds depend on the orbital radii of the electrons themselves, in our case, to obtain a visual image of the atom, as well as in Figure 11, we assume the radii of the electron clouds equal in magnitude to half of their orbital radii (Figure 12b). In other words, the dimensions of the 2*p*-electrons should be close to the diameters of the 2*s*-electrons, but in this case all the lower shells would be hidden from view and the resulting visual image of the atom could not be analyzed.

Also, Figure 12 clearly shows that 1*s*- and 2*s*-electrons for Z=4 and Z=10 have different ratios of the sizes of electron clouds. This is due to a change in the scale of representation of atoms, as well as due to disproportionate changes in the size of clouds at different atomic numbers.

Atomic numbers *Z=18* and *Z=36*. Let us now proceed to the consideration of subsequent atoms having completely closed subshells in the ground state. These include atoms containing the number of electrons: Z = 18 and Z = 36 (fig. 13).

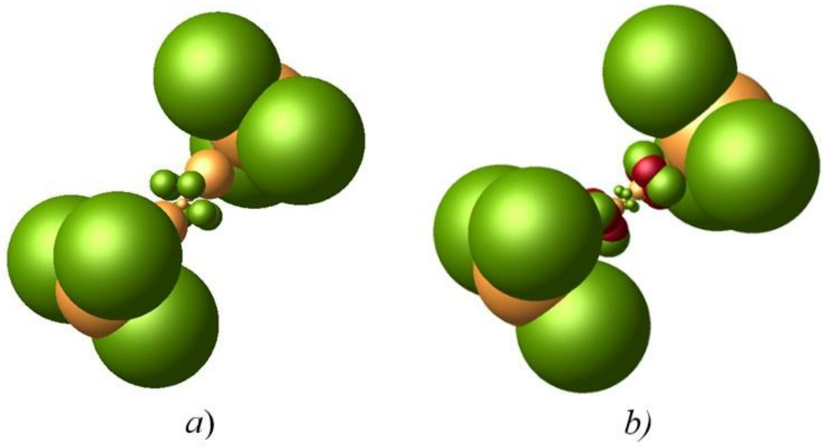


Fig. 13 Dimensional models for closed electron shells of an atom:
a) Z = 18; *b)* Z = 36

In the case of a closed electron shell of an atom with a charge number Z = 18, it is clearly seen that the main role is played by the electrons of the 3*p* subshell. Even the appearance of 3*d* electrons in an atom with Z = 36 practically did not affect the dominant position of 3*p* electrons.

Atomic numbers *Z=54* and *Z=86*. It is somewhat more difficult to determine the electron dispersal at Z = 54 and at Z = 86. So, 3*d* electrons "fall through" and are located near 2*p* electrons. Further, the dispersal of subsequent 4*f* electrons is also observed closer to the nucleus than that of the 4*s* and 4*p* electrons (Fig. 14).

As can be seen from the dimensional models of the electron shell of the atom, the positions of the *d*- and *f*-electrons are most deeply immersed in the atom. This phenomenon can be explained by a kind of "pushing apart" of electrons from nearby subshells, which allows *d*- and *f*-electrons to penetrate into deeper layers of the atom.

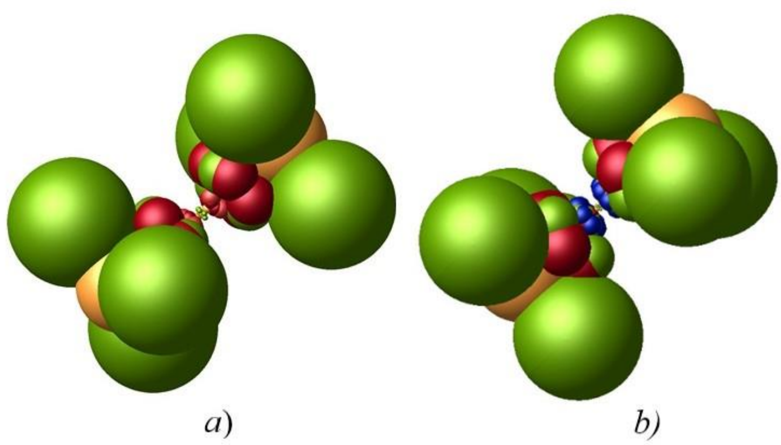


Fig. 14 Dimensional models of atomic electron shells:
a) Z = 54; *b)* Z = 86

Atomic number *Z=102.* A visual analysis of the dimensional model of the electron shell of an atom at Z = 102 (Fig. 15) shows that for a 7*s*-subshell, with an electron ionization energy of E_i (Z=102) = 6.66 M*eV*, the selection of an interval at which the ionization energy has a similar value for a 5*f*-subshell leads to the value: ΔR = 1.56$r_{\text{орб}}$.

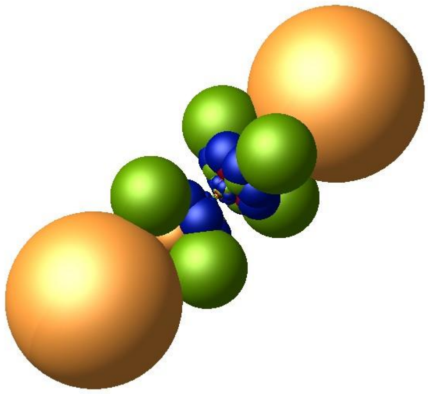


Fig. 15 Dimensional model of the electron shell of an atom at Z = 102

Even if *ns*-electrons are excluded from consideration, it can be seen that the general picture of the predominance of *np*-electrons, during the formation of electron shells, is preserved for almost the majority of atomic charge numbers.

4. CONCLUSION

In the present study, we have considered the spatial structure of the electron shell of an atom in the normal state. Particular attention was paid to the issue of visualization, as well as a new approach to determining a set of quantum numbers. We were also able to show that when considering the location of electron clouds, one can visually observe the "arrangement" of electrons near the nucleus of an atom, which will be of particular importance for the correct interpretation of theoretical and experimental data.

The proposed model of the atom electron shell is a kind of graphical extension of the shell model, since it makes it possible to represent the spatial structure of the atom as a set of shells consisting of electron clouds. The obtained results of the study allow us to conclude that using computer simulation, based on such parameters as the orbital radius and ionization energy, as well as quantum numbers; it is possible to visualize the spatial structure of the electron shell of the atom. Thanks to the visualization of the computer model, the properties exhibited by electrons in the atom and previously described as rules and principles become so obvious that they do not require postulation.

In this work, we focused on the possibility of visualizing and analyzing the structure of the electron shell of an atom. We have shown that the currently available set of principles and rules for the formation of the electron shell of an atom is sufficient to overcome the limitations imposed by the non-visibility principle [17].

The main results obtained in this study are as follows:

1. A method has been developed for computer simulation of the spatial structure of the electron shell of an atom, which includes a detailed presentation and justification of the proposed approach.
2. The concept of the basic quantum number is introduced, which makes it possible to expand the possibilities of describing the distribution of electrons in an atom.
3. A simple computer model has been developed that makes it possible to methodically and in a more convenient form show the application of the principles and rules responsible for the order of electron settlement in explaining the shell model of an atom.
4. The possibility of visualization of the spatial structure of the electron shell of the atom for the ground electronic state of the atom in the form of a dimensional computer model is shown.

The possibility of determining the spatial arrangement of electrons in individual subshells will allow, in the future, refining and expanding the methods and approaches used to study the electron shell of an atom.

References

1. Urusov B.C., Eremin N.N. Atomistic computer modeling. – M.: GEOS, 2012. – 428 p. (in Russian).

2. Eickerling G, Reiher M. The shell structure of atoms // J. Chem. Theory Comput. – 2008, no 4. – P. 286-296.

3. Smirnov B.M. Physics of atom and ion. – M.: Energoatomizdat, 1986. – 215 p. (in Russian).

4. Makagonov E.P. On the rules for filling shells of atoms and nuclei // Ural Mineralogical Collection. – 2008, No. 15. – pp. 3-8. (in Russian).

5. Condon E.U., Odabasi H. Atomic structure. – Lorid.: Cambridge: University Press, 1980. – 200 p.

6. Dmitrienko T.G. Physico-chemical fundamentals of materials science. – Saratov: SSTU Publishing House, 2012. – 851 p. (in Russian).

7. Potapov A.A. Electronic structure of atoms. – M: RCD, 2009. – 264 p. (in Russian).

8. Klechkovsky V.M. Distribution of atomic electrons and the rule of sequential filling of groups. – M.: Atomizdat, 1968. – 432 p.

9. Gillespie R.J. Molecular geometry – London: Van Nostrand Reinhold company, 1972. – 280 p.

10. Lucas J. A physical model for atoms and nuclei //Galilean Electrodinamics, January/February 1996. – Vol. 7, No. 1. – P. 3-12.

11. Parson A.L. A magneton theory of the structure of the atom: (with two plates) / Smithsonian Miscellaneous Collections. – 1915, Vol. 65, No. 11. – 80 p.

12. Langmuir J. The arrangement of elektrons in atoms and molecules / Physical Review. – 1919, 22. – P. 505-587.

13. Gryziński M.A. Collisions between systems of Coulomb particles. I. Small-angle scattering for time-dependent fields / J. Chem. Phys. – 1975, Vol. 62, No. 7. – P. 2610-2619.

14. Fano U., Fano L. Physics of atoms and molecules; an introduction to the structure of matter. – Chicago: University of Chicago Press, 1973. – 592 p.

15. Migal L.V., Bondarev V.G., Bondareva T.P. Computer modeling of parameters of the electronic shell of the atom // Research result. Information technologies. – 2021, T.6, №1. – P. 30-39.

16. The US Atomic Database: [Electronic resource]. Access mode: https://www.nist.gov/pml/productsservices/physical-reference-data / (accessed: 02.11.2021).

17. Heisenberg W. Der teil und das ganze: gespräche im umkreis der atomphysik. – Munchen: R. Piper & Co. Verlag, 1969. – 288 s.