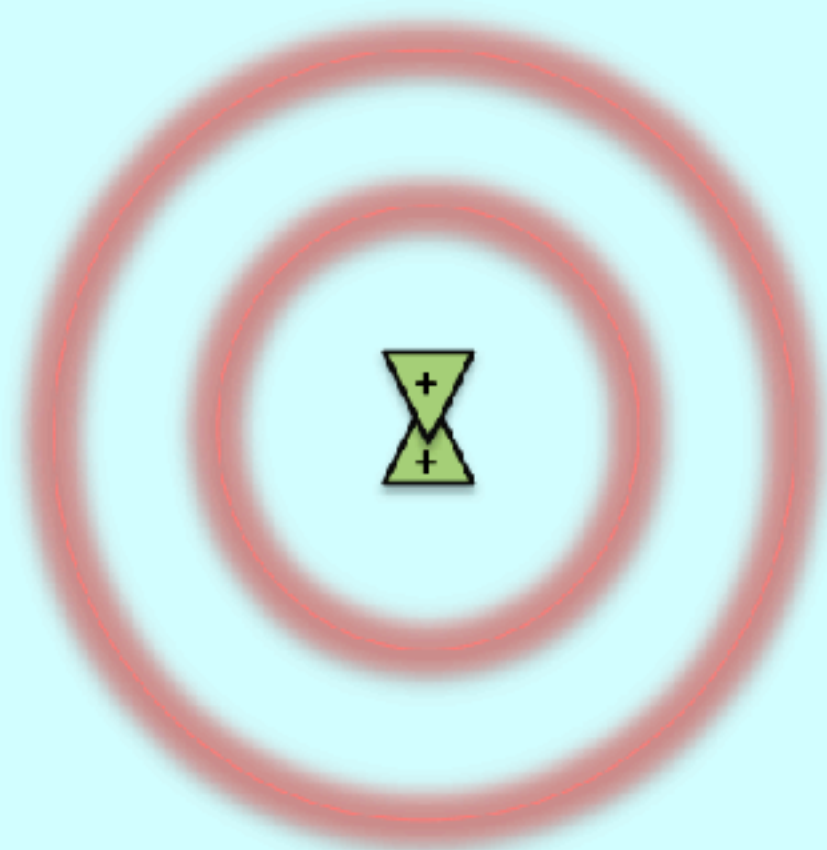


# The Atomic Structure of the Chemical Elements

Jozsef Garai



2026

The collection of the previous publications of the author offers a completely new description for the atomic structure of the chemical elements. The model rests on three major interrelated assumptions. One, the charge distribution of the nucleus must be invariant in order to reproduce the identical chemical characteristics of the elements. Two, classical electromagnetism is valid at atomic scale, and three, the opposite charges in the atoms are in static equilibrium. Built on these assumptions a new model for both the nucleus and the electronic structures are proposed. The main ingredients of the model are:

- protons and neutrons are arranged in a face centered cubic lattice in the nucleus
- expanding the basic unit of this lattice, a tetrahedron, reproduces the periodicity of the chemical elements
- the invariant chemical characteristics of the elements are ensured by the lattice arrangement of the unshielded protons
- the point charge free electron transfers to a surface charge when captured by the nucleus and vice versa

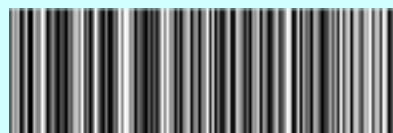
The formed surface charge electron shell around the nucleus complies with all the features of the atoms and offers a physical explanation for quantum mechanics, electronegativity and covalent bonds.



Prof. Jozsef Garai is retired from the University of Debrecen, Hungary. He earned his Ph.D. at Florida International University in Miami. His research includes: optical properties of diamonds; Equation of States; theoretical description of melting and vaporization; structure of the nucleus and the electron shell

of the atoms. Garai has more than 50 publications, which have been cited more than 500 times.

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# **The Atomic Structure of the Chemical Elements**

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Motto: Nature is simple and if you make it complicated you just fool yourself :)

## PREFACE

The basic building blocks of nature, and the basic constituents of chemistry are the atoms. According to Feynman (1961), the atomic theory is the most important concept in science. He raised the following question: “If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the most information in the fewest words? I believe it is the *atomic hypothesis* (or the *atomic fact*, or whatever you wish to call it) that *all things are made of atoms—little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another*. In that one sentence, you will see, there is an *enormous* amount of information about the world, if just a little imagination and thinking are applied.”

Atomic theory is the cornerstone of chemical sciences, offering an essential framework for understanding the composition, properties, and the behavior of matter. The current consensus on the atomic structure was formulated about a hundred years ago. It is timely to revisit these models in the enlightenment of the newly developed instrumentations and theories.

In the earliest days of science researchers were arguing philosophically what might be the reasonable explanation for an observed phenomenon. The majority of the contemporary science community claims that these arguments are useless because they do not add anything to our understanding of nature. The current consensus on the aim of science is that science collects facts (data) and discerns the order that exists between and among the various facts (e.g., Feynman 1985). According to this approach the mission of science is over when the phenomenon under investigation has been described. It is left to the philosophers to answer the question of what is the governing physical process behind the observed phenomenon. This approach goes back to Newton, when science was unable to offer a physical explanation for gravity. The same attitude is persisted by contemporary science, for the same reason, since nearly a century, after the development of quantum theory, there is still no consensus in the scientific community regarding the interpretation of the theory’s foundational building blocks (Schlosshauer et al. 2013).

The author believes that the description of an observed phenomenon is only the first step in our understanding of nature. The real essence of science should be to understand the physical processes governing the described phenomenon. Following this approach, an attempt is made here to reveal the structure of the atoms, and how this structure defines the fundamental chemical behavior of the elements. No advanced knowledge is required to read the book, but the presented arguments should be thought of carefully, and read it with an open mind.

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# **The Atomic Structure of the Chemical Elements**

# 1. History of the atomic theory

The hypothesis, all things are made of atoms is not new. The Greek philosopher Democritus proposed in the 5<sup>th</sup> century BCE that matter could be broken up into tiny indivisible parts, which cannot be divided further, and he called these smallest particles to atoms. His argument was, if a matter has been cut into half and this process is continued until you are unable to divide further and that matter is the atomos (indivisible). Aristotle disagreed, and he was citing Zeno's paradox, if you cut something into half you always get a half of something. Consequently, you would never get to zero. Thus, there is no limit in the cutting of matter. Nearly two thousand years Aristotle's view of matter was dominating and it was assumed that there were no building blocks of the matter.

Chemists at the very beginning of the nineteenth-century knew that there are elements and these elements cannot be produced from one to the other. John Dalton kept the name of atoms for the smallest particle but used for the chemical elements. He stated in 1803 that matter is composed of atoms, which are identical for a given element. Atoms of the different elements have different weights and combine in simple ratios to form compounds.

J.J. Thomson (1897) cathode ray experiment showed that the ray composed of negatively charged particles, whose mass is far less than the mass of any of the atoms used for the experiments. Thomson concluded that all atoms should consist of negatively charged particles, whose mass is much smaller than the atom itself. This discovery demonstrated that atoms are not the smallest fundamental units of nature. He called these negative subatomic particles to corpuscles, which is currently known as electrons. Atoms have an overall neutral charge. Thus, the negative charge of the electron/s must be counterbalanced by positive charge/s in the atoms.

Based on Earnshaw's theorem, point charges cannot be in stable stationary configuration solely under electrostatic interactions. The stability of the atoms then requires that the attractions of the point charge electrons should be balanced out by distributed positive charge/s. Thomson in 1904 proposed that the electrons should be floating in diffuse positive charge forming neutral atoms. This atom model is known as the "plum pudding" model (Fig. 1.1).

The discovery of radioactivity (Becquerel, 1896) emitting charged particles also indicated that atoms are built up from smaller particles. Radioactivity was explained as a spontaneous transmutation of the elements.

The first modern description of the atoms dates back to 1911. Hans Geiger and Ernest Marsden scattering experiments, bombarding a gold foil with alpha particles, showed that the positive charge in the atoms is very tiny; therefore, it should be considered as a point charge in the middle of the atom. The rest of the space inside the atom is empty. This positive charge, the nucleus, consists of almost the entire mass of the atom. Rutherford (1911), who supervised the experiments, suggested that electrons should be orbiting around the heavy nucleus and the attraction between the opposite charges should be balanced out by the centrifugal force of the orbiting electron/s.

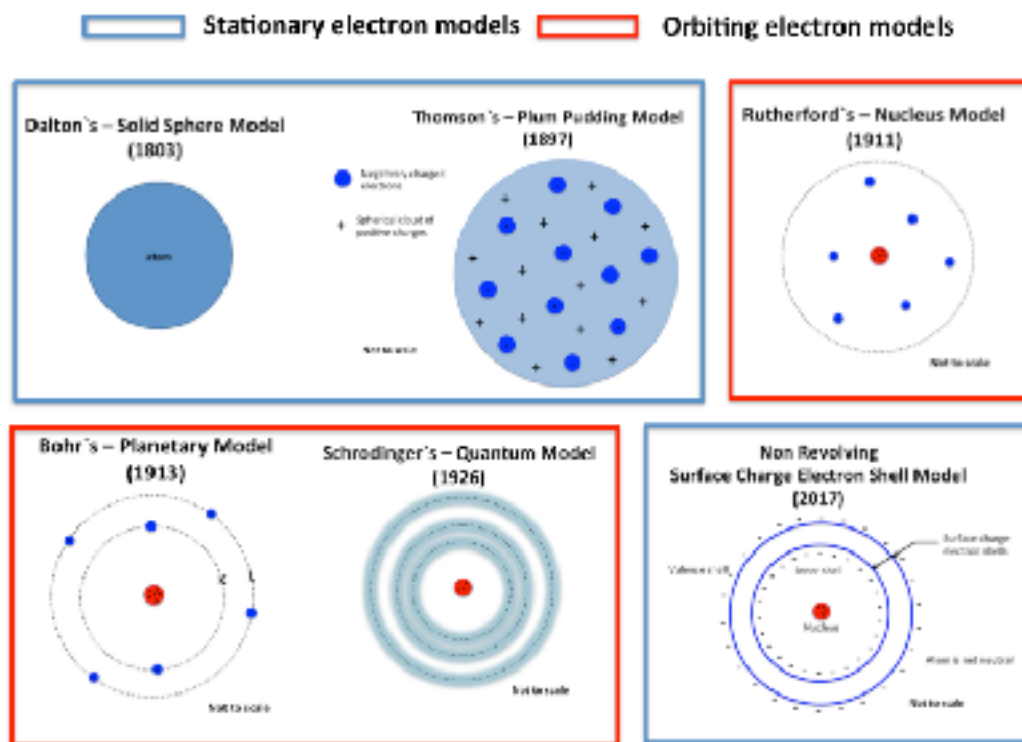
Bohr (1913) refined the Rutherford nucleus model by suggesting that the angular momentum of the orbiting electron should be discrete, and the multiple of the reduced Planck constant ( $\hbar$ ).

$$m_e v r = n \hbar \quad (1.1)$$

where  $m_e$  is the mass of the electron,  $v$  is the velocity of the electron,  $r$  is the radius of the orbit, and  $n$  is integer, called principal quantum number. Bohr's planetary model is able to reproduce the main emission lines of the hydrogen (Balmer 1885), derive the correct values for the Rydberg constant (1888), the radius of the hydrogen atom, and the ionization energy. Despite this enormous success, the model has many shortcomings (Baily 2013).

The currently accepted atom model employs the wave-particle duality of matter proposed by De Broglie (1924). This hypothesis had been confirmed by the experiments of Davisson and Germer (1927), which demonstrated the wave nature of the electron. This is the fundamental base of quantum mechanics, which uses the wave function to describe all the physical phenomena at atomic scale. The wave equation describing the particles had been proposed by Schrödinger (1926). This purely mathematical approach is able to reproduce not just the results of the Bohr's model but all the known features of the Hydrogen atom. After almost a hundred years there is still no consensus in the scientific community why this mathematical treatment is able to correctly describe the characteristic features of the electron (e.g. Connerade 2023). It works, so we just have to accept it...

This study investigates the atomic structure of the chemical elements. The atoms of each element have distinct chemical characteristics, which follow a pattern described by the periodic table. It is investigated what structural element of the atoms is responsible for the organizing principle and what is the underlying physics behind this pattern.



**Figure 1.1** Timeline of the atomic models. The proposed models can be divided into two major categories. One, stationary charge models, where the electrostatic stability of the opposite charges requires that one of the charges must be distributed. Two, the orbiting electron models, where the stability of the opposite charges is maintained by

the orbiting centrifugal force of the electron/s. The latest model, the non-revolving surface charge electron shell model, is discussed in chapters 7-9.

## References to Chapter 1

- Baily, C. Early atomic models – from mechanical to quantum (1904–1913). *Eur. Phys. J. H* **2013**, *38*, 1-38.
- Balmer, J. J. Notiz über die Spektrallinien des Wasserstoffs. in Verhandlungen der Naturforschenden Gesellschaft in Basel (Naturforschenden Gesellschaft, Basel, Vol. 7, p. 548-560 & 750-752 (1907); also in *Ann. Physik* **1885**, *25*, 80.
- Bohr, N. On the constitution of atoms and molecules. *Philos. Mag.* **1913**, *26*, 1-25; *ibid.* *26*, 476-502; *ibid.* *26*, 857-875.
- de Broglie, L. *Recherches sur la Théorie des Quanta*, PhD Thesis, Masson, Paris, 1924.
- Chadwick, J. Possible Existence of a Neutron. *Nature* **1932**, *129*, 312.
- Chadwick, J. The Existence of a Neutron. *Proc. R. Soc. London* 1932, *13*, 692-708.
- Connerade, J-P. The Atom at the Heart of Physics. *Atoms*, **2023**, *11*, 32.
- Davissson, C., & Germer, L.H. Diffraction of electrons by a crystal of nickel, *Phys. Rev.* **1927**, *30(6)*, 705-741.
- Dutailly, J.C. (2013). Quantum Mechanics revisited, arXiv:1301.0885 [math-ph].
- Earnshaw, S. On the nature of the molecular forces which regulate the constitution of the luminiferous ether. *Transaction of the Cambridge Philosophical Society* **1842**, *7*, 97-112.
- Feynman, R.P., Lectures on Physics, Vol. 1, Ch. 1 (Lectures presented at Caltech during 1961-64); <https://www.feynmanlectures.caltech.edu>
- Feynman R.P. (1985). QED, The Strange Theory of Light. Princeton University Press, Princeton, NJ.
- Rydberg, J.R. The Minutes of Society for Physics and Mathematics (Lund, Sweden) of November 5th, Showing Rydberg's Formula (University of Lund, Sweden, 1888).
- Rutherford, E. LXXIX. The scattering of  $\alpha$  and  $\beta$  particles by matter and the structure of the atom, *Philos. Mag. Ser.* **1911**, *6*, 669-688
- Schlosshauer, M., Kofler, J., Zeilinger, A. (2013). A snapshot of foundational attitudes toward quantum mechanics. arXiv:1301.1069 [quant-ph] (2013); *Stud. Hist. Phil. Mod. Phys.* *44*, 222–230.
- Schrödinger, E. An Undulatory Theory of the Mechanics of Atoms and Molecules, *Phys. Rev.* **1926**, *28*, 1049-1070.
- Schrödinger, E. Quantisierung als Eigenwertproblem (1st communication). *Annalen der Physik*, **1926**, *79*, 361–376. Reprinted in English in G. Ludwig, *Wave Mechanics*, Pergamon Press, London, 1988, p. 94–105.
- Thomson, J.J. (1904) On the structure of the atom: an investigation of the stability and periods of oscillation of a number of corpuscles arranged at equal intervals around the circumference of a circle; with application of the results to the theory of atomic structure, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, *7(5)* 237-265. <https://doi.org/10.1080/14786440409463107>

## 2. The Periodic Table\*

By 1860 about 60 elements had been identified, and this initiated a quest to find their systematic arrangement.

### 2.1 The emergence of the periodic table

Based on similarities, Döbereiner in 1829 suggested grouping the elements into triads. Newlands (1864) in England arranged the elements in order of increasing atomic weights and based on the repetition of chemical properties, proposed the “Law of Octaves”. Listing the elements also by mass, Mendeleev (1869; 1872) in Russia and Meyer (1870) in Germany simultaneously proposed a 17-column arrangement with two partial periods of seven elements each (Li-F and Na-Cl) followed by nearly complete periods (K-Br and Rb-I). Mendeleev gets greater credit for this discovery because he published the results first; he also rearranged a few elements out of strict mass sequence in order to fit better to the properties of their neighbors and corrected mistakes in the values of several atomic masses.

Additionally, he predicted the existence and the properties of a few new elements by leaving empty cells in his table. Mendeleev’s periodic table did not include the noble gasses, which were discovered later. Argon was identified by Rayleigh in 1895/a-b. The remaining noble gasses were discovered by Ramsey (1897) who positioned them in the periodic table in a new column. Anton van den Broek (1911; 1913) suggested that the fundamental organizing principle of the table is not the weight but rather the nuclear charge, which is equivalent to the atomic number. The extended 18-column table was slightly modified based on Moseley’s experiments (1913). He rearranged the table according to the atomic numbers. The discovery of the transuranium elements from 94-102 by Seaborg (1951) further expanded the table. He also reconfigured the table by placing the lanthanide/actinide series at the bottom. There is no “standard” or approved periodic table. The only specific recommendation of the International Union of Pure and Applied Chemistry (IUPAC), which is the governing body in Chemistry, is that the Periodic System of the Chemical elements (PSCE) should follow the 1 to 18 group numbering (Leigh, 2009) (Fig. 2.1).

### 2.2 Sequences of the Table

Investigating the organizing pattern of the PSCE it has been concluded that three sequences emerge from the periodic table (Garai, 2008). These sequences are the fundamental [ $S_{\text{fundamental}}$ ], the periodic [ $S_{\Delta Z}$ ], and the atomic number [ $S_Z$ ] sequences. The fundamental sequence of the table shows how many times the same number of elements in a period are repeated. This sequence consists of the number of periods with the same number of elements (Fig. 2.1).

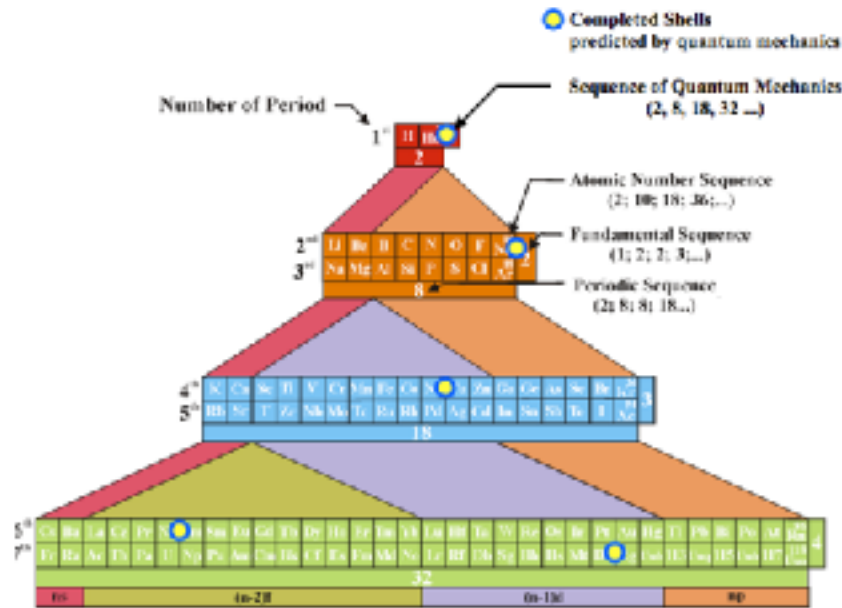
$$S_{\text{fundamental}} = \{ 1, 2, 2, 3, 3, 4, 4, \dots \} \quad (2.1)$$

The sequence of the number of elements  $[\Delta Z(n)]$  within the period or the length of the following periods can be defined as:

$$S_{\Delta Z} = \{ 2, 8, 8, 18, 18, 32, 32 \dots \}. \quad (2.2)$$

The atomic number or the nuclear charge of the elements  $[Z(n)]$  in a completely developed period follows the sequence

$$S_Z = \{ 2, 10, 18, 36, 54, 86, 118 \dots \}. \quad (2.3)$$



**Figure 2.1.** The sequences of the periodic table. The sequence derived from quantum theory is also shown. It can be seen that the sequence derived from quantum theory does not match with the sequences of the PSCE.

### 2.3 Pauli Exclusion Principle

In order to explain the observed light emission patterns observed in atoms, Pauli postulated the exclusion principle: “In an atom there cannot be two or more equivalent electrons for which the values of all four quantum numbers coincide. If an electron exists in an atom for which all of these numbers have defined values, then this state is occupied.” (Pauli, 1925; 1964). The principle was originally postulated for electrons but it has been generalized and now includes other particles. The Pauli Exclusion Principle is one of the cornerstones of quantum physics and thus it is at the basis of the foundation of modern physics. It is connected to spin statistics dividing the world into fermions and bosons. Particles with half-integer spin (fermions) are described by antisymmetric wave functions and particles with integer spin (bosons) are described by symmetric wave function (Pauli, 1946). The rise of the periodic table is one of the important outcomes of the Pauli exclusion principle.

Pauli in his Nobel lecture in 1946 (Pauli, 1946) stated that “I was unable to give a logical reason for the exclusion principle or to deduce it from more general assumptions. I always had the feeling and I still have it today, that this is a deficiency.” After many decades have passed, the physical explanation for Pauli’s postulate is still lacking (Kaplan, 2013). The Pauli exclusion principle is the theoretical basis for the periodic table. Consequently, the physical explanation for the periodicity of the chemical elements is also lacking. The current standing of the theoretical explanations are summarized.

## 2.4 Proposed Theoretical Explanations

The Aufbau principle, how the electronic configuration of the atoms is built up, was originally postulated by Niels Bohr and Wolfgang Pauli. They stated that “The orbitals of lower energy are filled in first with the electrons and only then the orbitals of high energy are filled.”. The energy levels calculated from the hydrogenic model, or the main quantum number, follow the sequence of  $2n^2$ . Only the first two entries of this quantum number sequence are consistent with the periodic table. In order to explain the periodic sequence by quantum theory the (n, l) rule or the Madelung energy ordering (Karapetoff, 1930; Madelung, 1936) has been suggested, which applies to neutral atoms in their ground state. The majority of general and physical chemistry books present the symmetry of the PSCE as satisfactorily explained by either the electronic structure of the elements (Bohr, 1922; Hund, 1925; Slater, 1930; Condon, 1935; Landau & Lifschitz, 1977; Schwabl, 2001; Atkins & Atkins, 2001) or by quantum mechanics (Hartree, 1957; Fischer, 1977; Johnson, 2005). Some authors present a quantum justification of the rule (Demkov and Ostrovsky, 1971; Ostrovsky, 1981, 2001). Not all of the elements comply with the (n,l) rule; therefore, general acceptance is lacking (Scerri 2004; Boeyens, 2008). Based on the conflicting interpretations it can be concluded that the most important periodic sequence of the chemical elements has not been satisfactorily explained (Scerri, 1998; Schwartz and Wang, 2010; Boeyens, 2013). One example might be the positions of Hydrogen and Helium. Hydrogen has one 1s electron but also one electron is needed to attain inert configuration. Thus it can be either placed in the 1<sup>st</sup> group or in the 17<sup>th</sup> group. Based on chemical behavior, Hydrogen is neither halogen nor alkali metal but rather both. Thus the position of Hydrogen in the PSCE is uncertain (Scerri, 2007). Helium with its 1s<sup>2</sup> electron configuration is the other element with uncertain position. Helium should be in the 2<sup>nd</sup> group. However, based on its chemical properties equivalent to an inert gas, it is placed into group 18. Besides Helium, the outermost electron configuration of group 18<sup>th</sup> is 2p<sup>6</sup>. No theoretical explanation for the shift in the electron configuration from 2p<sup>6</sup> to 1s<sup>2</sup> or vice versa is offered. The proposed theoretical explanations for the periodicity of the chemical elements are incomplete. It has been suggested by many authors that quantum mechanics is unable to explain the most important aspects of the periodic table (Scerri, 1998; Boeyens, 2008; Schwartz and Wang, 2010; Boeyens, 2013). The substantial number of articles in the current literature (e.g. Sneath, 2000; Giunta, 2001; Kragh, 2001; Ostrovsky, 2001; Scerri 2001; Dudek et al. 2002; Baum, 2003; Ostrovsky, 2003; Moore, 2003; Scerri, 2003; Friedrich, 2004; Kibler, 2004; Schunck & Dudek, 2004; Scerri, 2004; Schwarz, 2004; Rouvray & King, 2005; Bent, 2006; Rouvray & King, 2006 ; Wang, 2006; Restrepo & Pachon 2007; Schwarz, 2007; Weinhold & Bent, 2007; Boeyens &

Levendis, 2008; Wang & Schwartz, 2009) discussing the fundamental problems of the PSCE nearly one-and-a-half centuries after its invention indicates that the complete physical understanding of the symmetry expressed by the PSCE is still lacking.

Despite the remaining outstanding questions, there is a general agreement that the elements should be arranged in an increasing atomic number order in the PSCE. The symmetry relating to the nuclear charge is invariant in the PSCE.

## 2.5 Consequences of the Pauli Exclusion Principle

The chemical properties of the elements are defined by the electronic structure of the outermost or valence shell. The identity of an atom, including its electronic structure is determined by the nucleus or more specifically by the number of protons (Broek, 1911, 1913). The interaction between the atomic particles in stationary positions can be described as:



The negatively charged electrons in an atom are captured by the electrostatic attraction of the positively charged protons. The electrostatic attraction between the two differently charged particles is described by an inverse square law. The attraction between a proton and a captured electron is the function of the distance between the two charges. The energy of a captured electron in its ground state depends on the distance between the two particles. Electrons with different energies in their ground states should be separated by different distances from the protons capturing them. This distance must be invariant, otherwise the electronic structure of the elements would not be invariant. In order to maintain the configuration of the protons and the distances between the protons and the captured electrons, the position of the protons must be invariant. This condition requires a lattice arrangement of the nucleon. The lattice structure of the nucleus ensures that if a lattice is occupied then another proton cannot have the same position. Thus the nuclear lattice model offers a feasible physical explanation for the Pauli Exclusion Principle, which requires that the protons in the nucleus cannot co-exist in the same location. In order to comply with the Pauli Exclusion Principle the protons in the nucleus must have a lattice arrangement.

## References to Chapter 2

This chapter was published in the book of Mendeleev to Oganesson. A Multidisciplinary Perspective on the Periodic Table in 2018.

\*Garai, J., Nuclear lattice model and the electronic configuration of the chemical elements, in Mendeleev to Oganesson. A Multidisciplinary Perspective on the Periodic Table, Edited by Eric Scerri and Guillermo Restrepo, Oxford University Press (2018)

Atkins, F.P., Atkins J.P.: Physical Chemistry, 7th Ed.; Oxford University Press (2001)

- Baum, R. M.: Celebrating the Periodic Table, Chem Eng News **81**, 28-29 (2003)
- Bent, H.: New Ideas in Chemistry from Fresh Energy for the Periodic Law. AuthorHouse: Bloomington, IN (2006)
- Boeyens, J.C.A.: Chemistry from First Principles, Springer Science and Business Media B.V. (2008)
- Boeyens, J. C. A., Levendis, D. C.: Number Theory and the Periodicity of Matter; Springer: Dordrecht (2008)
- Boeyens, J.C.A.: The Chemistry of Matter Waves, Springer (2013)
- Broek, A: The Number of Possible Elements and Mendeléeff's "Cubic" Periodic System. Nature, 1911, **87**, 78 (1911)
- Broek, A: Intra-atomic Charge. Nature **92**, 372-373 (1913)
- Bohr, N.: The Theory of Atomic Spectra and Atomic Constitution; Cambridge University Press (1922)
- Condon E.U., Shortley, G.H.: The Theory of Atomic Spectra; Cambridge University Press (1935)
- Demkov, Y. N., Ostrovsky, V.N.:  $n + 1$  filling rule in the periodic system and focusing potentials. Zh. Eksp. Teor. Fiz. **62**, 125-132 (1971); Errata **63**, 2376 (1972); Sov. Phys.-JETP **35**, 66-69 (1972)
- Döbereiner, J.W.: Versuch einer Gruppierung der elementaren Stoffe nach ihrer Analogie, Pogg. Ann. Phys. Chem. **15**, 301-307 (1829)
- Dudek, J., Gozdz, A., Schunck, N.; Miskiewicz, M.: Nuclear Tetrahedral Symmetry: Possibly Present throughout the Periodic Table. Phys. Rev. Lett. **88**, 252502 (2002)
- Fischer, C.F.: The Hartree-Fock Method for Atoms. A Numerical Approach. Wiley-Interscience (1977)
- Friedrich, B.: Hasn't it? A commentary on Eric Scerri's paper "Has quantum mechanics explained the periodic table?" Fund. Chem. **6**, 117-132 (2004)
- Garai, J.: Mathematical Formulas Describing the Sequences of the Periodic Table, International Journal of Quantum Chemistry **108**, 667-670 (2008)
- Giunta, C.J.: Argon and the Periodic System: The Piece that would not fit. Fund. Chem. **3**, 105-128 (2001)
- Hartree, D.R.: Proceedings of the Cambridge Philosophical Society **24**, 89-132 (1928); The calculation of atomic structures. Wiley (1957)
- Hund, F.: Concerning the interpretation of complex spectra, especially the elements scandium to nickel, Zeitschrift für Physik **33**, 345-371 (1925)
- Johnson, R.D.: NIST Computational Chemistry Comparison and Benchmark Database, NIST Standard Reference Database, 101 (2005)
- Kaplan, I.G.: Exclusion Principle. Can It Be Proved? Found. Phys. **43**, 1233-1251 (2013)
- Karapetoff, V.: A Chart of Consecutive Sets of Electronic Orbits within Atoms of Chemical Elements. Journal of Franklin Institute **210**, 609-614 (1930)
- Kibler, M.R.: Classifying Chemical Elements and Particles. In Rouvray D.H. and R.B. King (Eds.), The Periodic Table: Into the 21st Century, ch. 11, pp. 297-329 (2004)
- Kragh, H.: The first subatomic explanation of the periodic system. Fund. Chem. **3**, 129-143 (2001)
- Landau, L.D., Lifschitz, L.M.: Quantum mechanics; Pergamon Press (1977)
- Leigh, J.: Periodic Tables and IUPAC. Chemistry International IUPAC, **31**, 1 (2009)
- Madelung, E.: Die Mathematischen Hilfsmittel des Physikers, 3rd edn., Berlin: Springer, p. 359 (1936); 6th edn., Berlin, p. 611 (1950)
- Mendelejev, D.: Ueber die Beziehungen der Eigenschaften zu den Atomgewichten der Élemente, Z. Chem. **12**, 405-406 (1869); abstracted and translated into German from Zhur. Russ. Fiz. Khim. Obshch. **1**, 60-77 (1869)
- Mendelejev, D.: Die periodische Gesetzmässigkeit der chemischen Élemente, Ann. Chem. Pharm., 1872, Suppl. **8**, 133-229 (1872)
- Meyer, L.: Die natur der chemischen Elemente als Function ihrer Atomgewichte, Ann.. Supplementband, VII. pp. 351-64 (Heft 3) (1870)
- Moore, J. W.: Modern Quantum Look at the Periodic Table of Elements. In Brändas, E. and Kryachko, E.S. (Eds.), Fundamental World of Quantum Chemistry. Vol. 2 , pp. 631- 674 (2003)

- Moseley, H.G.J.: The High-Frequency Spectra of the Elements. *Phil. Mag.* **26**, 1024–1034 (1913)
- Newlands, J.A.R.: On Relations Among the Equivalents, *Chem. News.* **10**, 94-95 (1864)
- Newlands, J. A. R.: On the Law of Octaves, *Chem. News.* **12**, 83 (1865)
- Ostrovsky, V.N.: Dynamic symmetry of atomic potential. *Journal of Physics B* **14**, 4425-4439 (1981)
- Ostrovsky, V.N.: What and How Physics Contributes to Understanding the Periodic Law. *Found. Chem.* **3**, 145–182 (2001)
- Ostrovsky, V.N.: Physical Explanation of the Periodic Table. *Ann. N.Y. Acad. Sci.* **988**, 182–192 (2003)
- Pauli, W.: *Collected Papers*, 2 vols. Interscience, New York (1964)
- Pauli, W.: Exclusion principle and quantum mechanics. Nobel Lecture, December 13, (1946)
- Ramsay, W.: An Undiscovered Gas. Report of the 67th Meeting of the British Association for the Advancement of Science 593–601 (1897)
- Rayleigh, L.: Argon. *Royal Institution Proceedings* **14**, 524–538 (1895/a)
- Rayleigh, L., Ramsay, W.: Argon, A New Constituent of the Atmosphere. *Philosophical Transactions* **186A**, 187-241 (1895/b)
- Restrepo, G., Pachon, L.: Mathematical Aspects of the Periodic Law. *Fund. Chem.* **9**, 189-214 (2007)
- Rouvray, D. H., King, R. B.: Eds. *The Mathematics of the Periodic Table*; Nova Science: New York (2006)
- Scerri, E.R.: How Good is the Quantum Mechanical Explanation of the Periodic Table? *J. Chem. Ed.* **75**, 1384-1385 (1998)
- Scerri, E.R.: The Periodic Table: The Ultimate Paper Tool in Chemistry. In Klein (Eds.), *Tools and Modes of Representation in the Laboratory Sciences*, pp. 163–177. Dordrecht: Kluwer Academic (2001)
- Scerri, E.R.: Löwdin's Remarks on the Aufbau Principle and a Philosopher's View of ab initio Quantum Chemistry. In Brändas, E. and Kryachko, E.S. (Eds.), *Fundamental World of Quantum Chemistry*, Vol. 2, pp. 675–694. Dordrecht: Kluwer (2003)
- Scerri, E.R.: The Best Representation for the Periodic System: the Role of the  $n+l$  Rule and of the Concept of an Element as a Basic Substance. In: D H, King R B, (Ed.), *The Periodic Table: Into the 21st Century*, Ch. 5. Baldock: Research Studies Press/IoP (2004)
- Scerri, E.R.: *The Periodic Table. Its Story and Its Significance*; Oxford University Press: Oxford (2007)
- Schunck, N., Dudek, J.: Nuclear tetrahedral symmetry *Int. J. Modern. Phys. E-Nucl. Phys.* **13**, 213-216 (2004)
- Schwabl, F.: *Advanced Quantum Mechanics*; Springer (2001)
- Schwarz, W.H.E.: Towards a Physical Explanation of the Periodic Table (PT) of Chemical Elements. In E.J. Brändas and E.S. Kryachko (Eds.), *Fundamental World of Quantum Chemistry*, Vol. **3**, pp. 645–669. Dordrecht: Kluwer, (2004)
- Schwartz, W.: Recommended Questions on the Road towards a Scientific Explanation of the Periodic System of Chemical Elements with the Help of the Concepts of Quantum Physics, *Found. Chem.* **2**, 139-188 (2007)
- Schwarz, W.H.E., Wang, S-G.: Some Solved Problems of the Periodic System of Chemical Elements. *Int. J. Quantum Chem.* **110**, 1455–1465 (2010)
- Seaborg, G.T.: The Transuranium Elements: Present Status Nobel Lecture 1951, December 12.
- Slater, J.C.: Atomic Shielding Constants, *Phys. Rev.* **36**, 57–64 (1930)
- Sneath, P.H.A.: Numerical Classification of the Chemical Elements and its relation to the Periodic System. *Fund. Chem.* **2**, 237-263 (2000)
- Wang, S.G., Qiu, Y.X., Fang, H., Schwarz, W.H.E.: The Challenge of the So-Called Electron Configurations of the Transition Metals. *Chem. Eur. J.* **12**, 4101–4114 (2006)
- Wang, S. G., Schwarz, W. H. E.: Icon of chemistry: the periodic system of chemical elements in the new century. *Angew Chem Int Ed* **48**, 3404-34-15 (2009)

Weinhold, F. J., Bent, H.A.: News from the Periodic Table: An Introduction to "Periodicity Symbols, Tables, and Models for Higher-Order Valency and Donor–Acceptor Kinships". *Chem Educ* **84**, 1145 (2007)

### 3. Nuclear Lattice Model\*

The nuclei have been identified by the scattering experiments of Hans Geiger and Ernest Marsden, carried out under the supervision of Rutherford. Ever since then this tiny center of the atom has been targeted by better and better penetrating probes to reveal its physics. Despite the great amount of knowledge that has been gathered about the properties of the atomic nuclei even the phase of the nucleus remains an enigma. The developed models, shell, liquid drop and cluster assume a gas, liquid and semi-solid phase for the nucleus respectively.

#### 3.1 Nuclear models

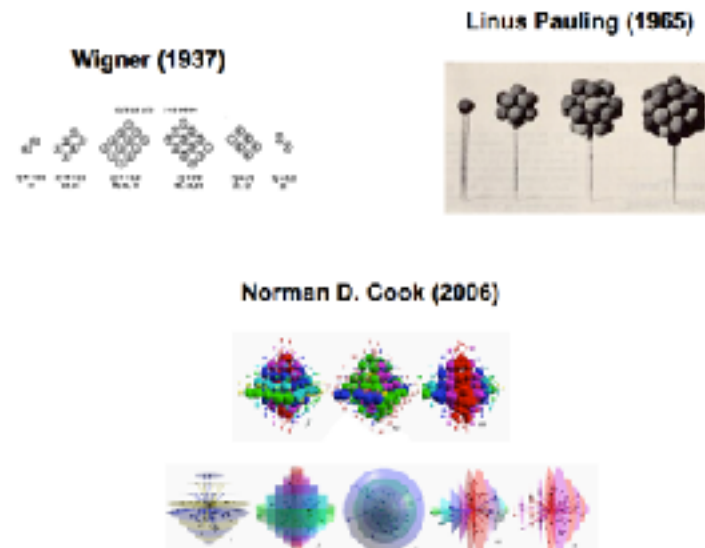
The most widely accepted models for the nucleus are: the shell (Mayer, 1949; Haxel et al., 1949; Rainwater, 1950; Mayer & Jensen, 1955), the liquid drop (Bohr, 1936; Feenberg, 1947) and the cluster (Hafstad & Teller, 1938) models. The shell model assumes a gas phase (Fermi) for the nucleus and is able to explain the independent quantum characteristics of the nucleons. The liquid drop model is able to explain the observed saturation properties of the nuclear forces, the low compressibility of the nucleus, the well-defined nuclear surface, the binding energies and most importantly the fission phenomena. The clustering of the alpha particle model was deduced from the fact that certain large nuclei emit alpha particles and the stability and the abundance of the  $4n$ -nuclei are significantly higher. These models are able to successfully describe certain selected properties of the nucleus; however, none of them are able to give a comprehensive description. The basic assumptions of the models are contradictory; therefore, it is impossible to combine them and develop a hybrid model.

The assumed phase of the nucleus in these models is gas, liquid or semi-solid. None of these phases have an invariant nucleon position; therefore, these models cannot maintain the invariant symmetry present in the Periodic System of the Chemical Elements. The preservation of symmetry requires a “solid phase” nucleus, in which the positions of the nucleons are preserved. “Solid phase” or lattice models have not been considered for many decades as a viable option because of the uncertainty principle and the lack of diffraction. In the 1960s, the discovery of quarks and neutron star research satisfactorily answered these objections and opened the door for lattice models. The first nuclear lattice models were presented by Linus Pauling in 1965/a-c.

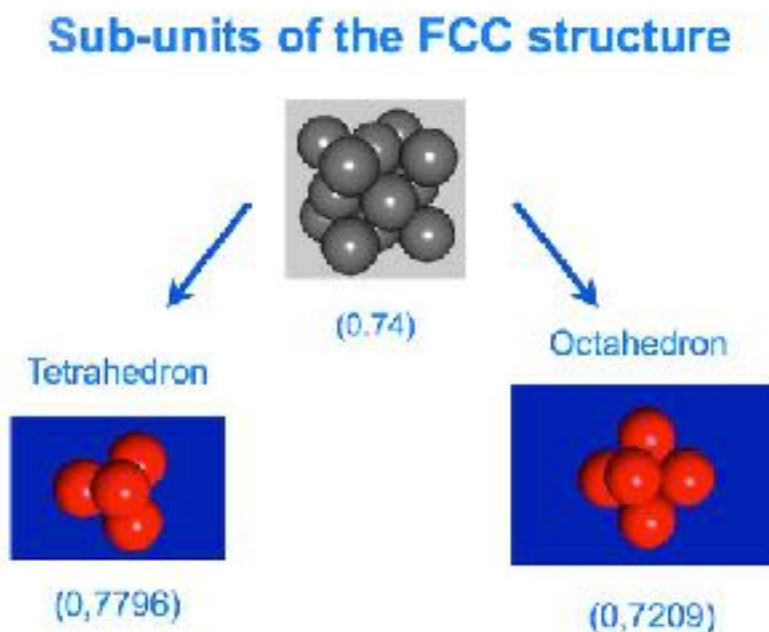
The lattice models can easily reproduce the various shell, liquid-drop, and cluster properties (Cook & Dallacasa, 1987; Cook & Hayashi, 1997). Asymmetric fission and heavy-ion multi-fragmentation are some of the phenomena that the traditional models of nuclear structure theory cannot explain, yet can be reproduced by lattice models (Gupta et al., 1996; 1997).

Significant effort has been made to find correlation between lattice positions and quantum numbers with partial success for FCC structure (Pauling, 1965/d; Cook & Dallacasa, 1987). The symmetries of Schrödinger’s equation also correspond to FCC geometry (Wigner, 1937). The common features of the developed lattice models are

that the protons and the neutrons have the same size and that they are alternately arranged in the closest packing array (Anagnostatos,1973; Canuto & Chitre, 1974; Lezuo, 1974; Cook, 1976; Matsui et al., 1980; Dallacasa, 1981). These assumptions are reasonable.



**Figure 3.1** Previous lattice models of the nucleus. These investigations expanded the FCC nuclear lattice structure spherically.



**Figure 3.2** The subunits of the face centered cubic structure and their densities. The density of the FCC structure is 0.74. The density of the sub-units, tetrahedron and octahedron are 0.7796 and 0.7209 respectively. Nuclear lattice model should expand these basic units. Tetrahedron is favored by the length of the first period, the alpha particle decay and the higher density.

The radii of protons and the neutrons differ only slightly (Schery et al., 1980). The same proton and neutron magic numbers indicate the same structural development for both protons and neutrons, which is consistent with an alternate arrangement. The equal spheres will most likely utilize the available space in the most efficient way, which is a closest packing arrangement. Previous investigations (Pauling, 1965/d; Cook & Dallacasa, 1987), which expanded the FCC structure spherically, had partial success in finding correspondence between lattice positions and quantum states (Fig. 3.1). The structure of the closest packing arrangements consists of tetrahedron and octahedron sub-units exclusively. In order to look for structural symmetry patterns built up in the FCC lattice, the expansion of these sub-units should be investigated (Garai, 1999; 2003) (Fig. 3.2).

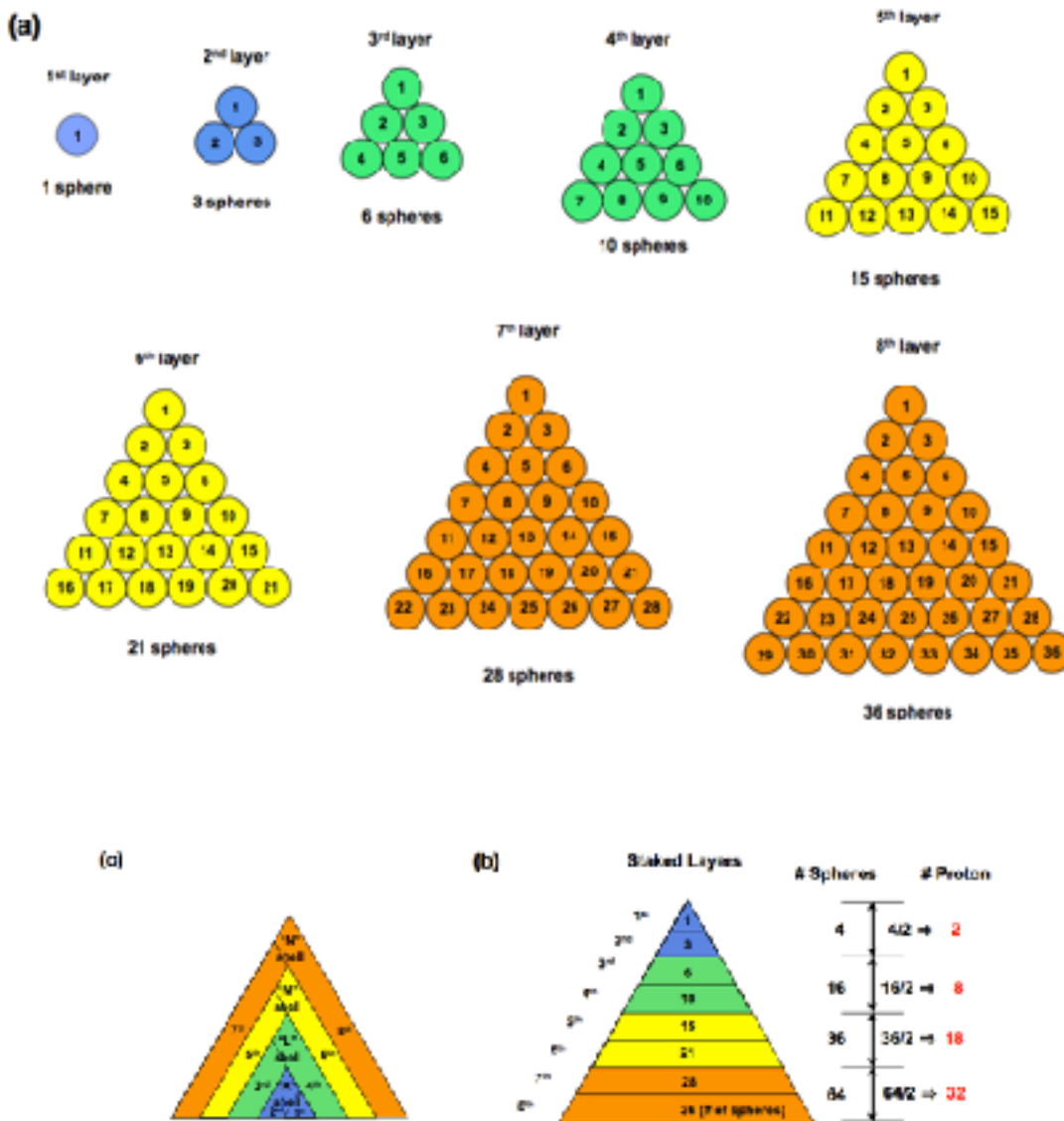
### 3.2 Tetrahedron FCC Lattice Model

Assuming that the bonding energy correlates with the nucleon density, then the densest structure should be formed preferentially. The densities of the tetrahedron and octahedron units in FCC are 0.7796 and 0.7209 respectively (Garai, 2010). The higher nuclear density indicates preferential tetrahedron formation. This formation is also supported by the length of the first period and the alpha particle decays.

The first sequence of the nuclear structural development is completed by the nucleus of Helium, which contains four nucleons. The closest packing arrangement of the four nucleons is a tetrahedron. Forming a tetrahedron sub-unit nucleus in the first completed period is an additional support for tetrahedron nucleus formation. Calculations of potential models, constrained by the hadron spectrum for the confinement of the relativistic quark (Goldman et al. 1988; Maltman et al. 1994) and the colored quark exchange model (Robson, 1978), are also consistent with a tetrahedron forming the He nucleus. The expansion of this tetrahedron seed of four nucleons is investigated here.

The tetrahedron arrangement of equal spheres in FCC packing can be formed from layers of equilateral triangles packed in two dimensional closest packing arrangement as shown in Fig. 3.3/a. Starting with one sphere and increasing the length of the side of the triangles by one additional sphere, the number of nucleons in each triangle plane will be 1, 3, 6, 10, 15, 21, 28, 36... (Fig. 3.3/a). Stacking these layers, the numbers of spheres in two consecutive layers are 4, 16, 36, 54... Assuming that protons and neutrons are alternately arranged in the lattice the number of spheres should be divided by two. This gives the proton numbers to 2, 8, 18, 32... respectively (Fig. 3.3/b). These numbers are identical with the number of elements in one row of the periodic table. If the tetrahedron is extended on two faces, then a shell-like structure can be formed (Fig. 3.3/c), which is consistent with the physical interpretation of the principle quantum number.

Investigating how many spheres can be accommodated in one row in the outer shell gives the total number of spheres in one row of 4, 12, 20, 28..., which corresponds to 2, 6, 10, 14... proton numbers (Fig. 3.4/a). These proton numbers are identical with the number of states determined by the angular momentum quantum numbers corresponding to s, p, d and f orbitals. The rows in the outer layers of the tetrahedron are one unit distance away from each other; thus the identical agreement of the number of nucleons with the angular momentum quantum numbers is not only in numerical agreement but also bears the same physical meaning defined by quantum theory.



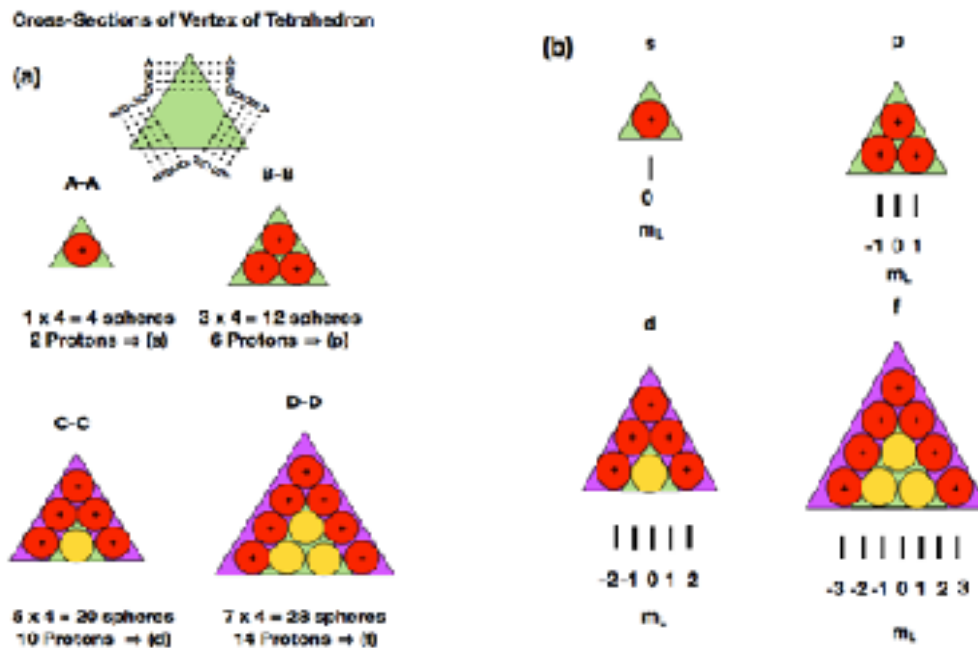
**Figure 3.3.** Representing both protons and neutrons with equal spheres and arranging them in FCC structure, the number of protons in the outer layers of a tetrahedron formation is the same as the number of possible states of the principal quantum numbers.

(a) The number of spheres in a two dimensional close packing arrangement in equilateral triangles.

(b) The number of spheres in two consecutive layers of the tetrahedron formation. Assuming a proton-neutron ratio of one, the outer layers of the tetrahedron contain the same number of protons as predicted by quantum theory.

(c). The same tetrahedron formation can be developed by adding the new layers to alternate sides.

The number of different positions of protons in one row of the outer shell is the same as the number of magnetic quantum numbers (Fig. 3.4/b). The lattice positions also reproduce the multiplicities. Thus the number of positions in an FCC lattice is identical with the quantum numbers if a tetrahedron seed is expanded. The lattice positions not only reproduce all of the quantum numbers but also bear the same physical meaning.



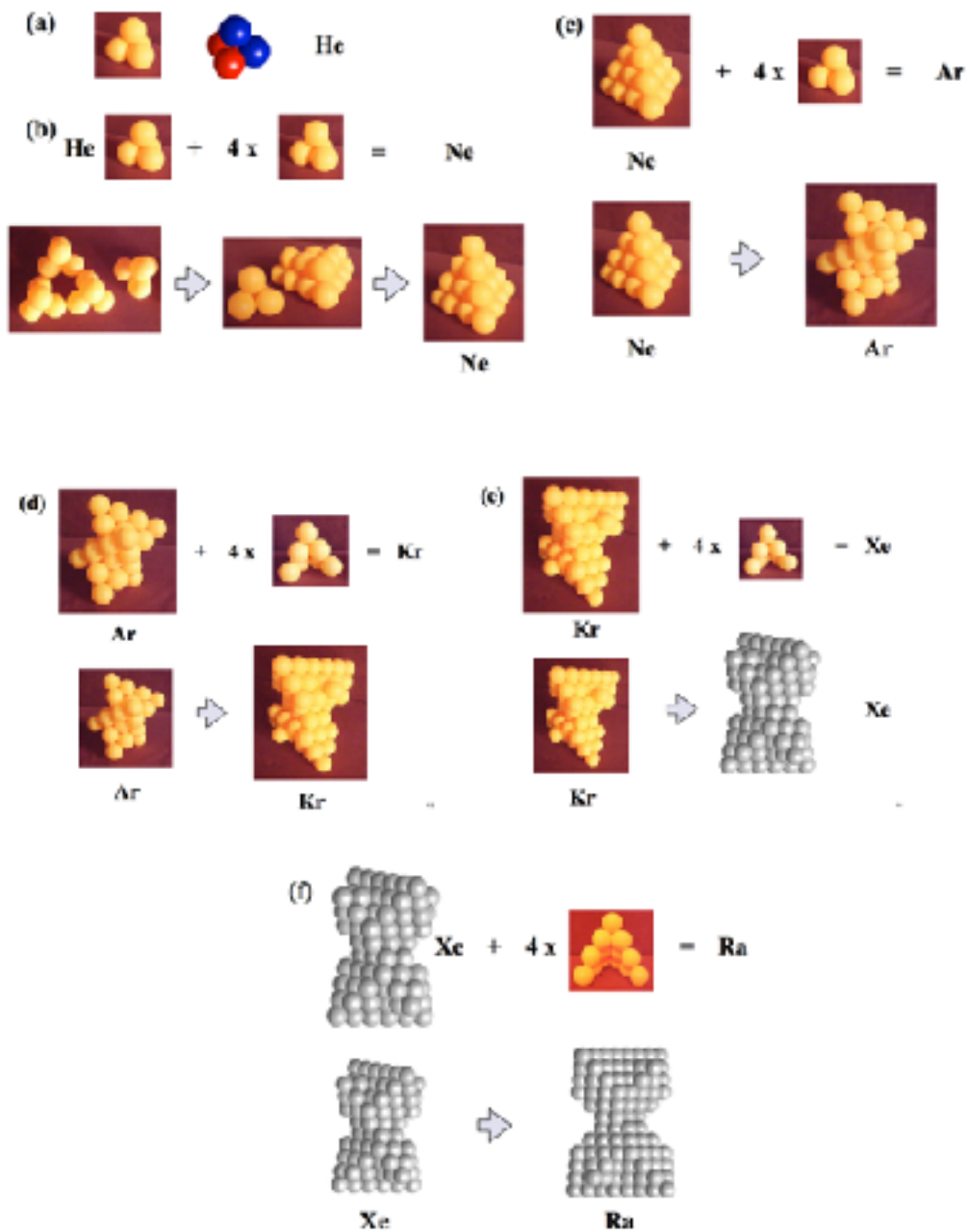
**Figure 3.4.** If a tetrahedron has been developed from a core tetrahedron, which contains four spheres, then the number of protons in one layer of the outer shell of the tetrahedron is equivalent with the number of states of the angular momentum quantum number or the corresponding sub-shell. The number of different positions of the protons in one layer of the shell is the same as the number of magnetic quantum numbers. The red circles represent the outer shell nucleons. The tetrahedron has four vertices; therefore, the number of spheres is multiplied by four.

(a) Number of spheres in one layer of a vertex of the tetrahedron.

(b) Number of the different proton positions in one layer of a vertex of a tetrahedron.

It has been assumed that a higher nuclear density is preferable to lower ones. The density of structures built in FCC arrangement can be described by the ratio of the tetrahedron and octahedron sub-units. The higher ratio corresponds to higher nuclear density. It can be shown that if a tetrahedron is expanded by rotating 90 degrees at each expansion, then the density of this joint or double tetrahedron is higher in comparison to a single tetrahedron. Based on the higher nucleons density it is suggested that the initial single tetrahedron should be developed by alternately rotating 90 degrees at each expansion of the tetrahedron. Three dimensional images of the completed tetrahedrons corresponding to the elements He, Ne, Ar, Kr, Xe and Ra are shown in Fig. 3.5/a-f. The nuclear FCC tetrahedral lattice structure expanded

by rotating 90 degrees reproduces not only the quantum numbers but also the periodicity of the chemical elements.



**Figure 3.5.** 3D images show the completed nuclear structures of the noble gases. (a) Helium (b) Neon (c) Argon (d) Krypton (e) Xenon (f) Radon

The additional characteristics of the nucleus, which are supporting the double tetrahedron nuclear lattice model are listed here:

- The expansion of the tetrahedron into four dimensions with angles of 109.5 degrees reproduces the original tetrahedron symmetry for every fourth nucleus. This is consistent with the observed zero magnetic momentum for each even-even nucleus.

- The disintegration of a structure should produce fragments of its basic lattice. The fragmentation of the tetrahedron FCC nuclear lattice is consistent with nuclear fission. The preferred alpha decay of the nuclear structure is consistent with the disintegration of an FCC lattice, which is built up from tetrahedron sub-units.
- The measured bulk density of the nucleus is consistent with the density of the FCC lattice arrangement (Cook and Dallacasa, 1987; Cook, 2010).
- The charge density distribution of the individual elements (Hofstadler, 1961) is consistent with the shape of the “double” tetrahedron FCC nuclear model.
- The double peak character of nuclear fission (e.g. Kienzler & Geckeis, 2018) is consistent with the double tetrahedron nuclear structure. If a thermal neutron with low energy hits the nuclear structure then the double tetrahedron structure in case of Uranium should be fragmented along its weakest surface into two unequal parts. Uranium 236 in highly excited states typically fragmented to Xe ( $Z=54$ ) a symmetrical, completed nuclear structure, and the remaining of the fragments forms a Sr ( $Z=38$ ). Higher energy excitation of the neutrons diminish the double peak character of the fission, which becomes single-humped (e.g. Zohuri, 2019). At higher energies the nucleus does not necessarily break along the weakest cross section and as the energy increases the nucleus fragmenting more and more into two equal parts.

### References to Chapter 3

This chapter was published in the book of Mendeleev to Oganesson. A Multidisciplinary Perspective on the Periodic Table in 2018.

\*Garai, J., Nuclear lattice model and the electronic configuration of the chemical elements, in Mendeleev to Oganesson. A Multidisciplinary Perspective on the Periodic Table, Edited by Eric Scerri and Guillermo Restrepo, Oxford University Press (2018)

Anagnostatos, G.S.: The Geometry of the Isomorphic Model of the Closed-Shell Nuclei. *Can. J. Phys.* 51, 998-1011 (1973)

Bohr, N.: Neutron Capture and Nuclear Constitution *Nature* 137, 344-348 (1936)

Canuto, V., Chitre, S.M.: Crystallization of dense neutron matter. *Phys. Rev. D*, 9, 1587-1613 (1974)

Cook, N.D.: An FCC Lattice Model For Nuclei. *Atomkernenergie* 28, 195-199 (1976).

Cook, N.D., Dallacasa, V.: Face-centered-cubic solid-phase theory of the nucleus. *Phys. Rev. C* 35, 1883-1890 (1987)

Cook, N.D., Hayashi, T.: Lattice models for quark, nuclear structure and nuclear reaction studies. *J. Phys. G: Nucl. Phys.* 1997, 23, 1109-1126 (1997)

Cook, N.D.: *Models of the Atomic Nucleus*, Springer, 2<sup>nd</sup> Ed. (2010)

Dallacasa, V: FCC (Face Centered Cubic) Lattice Model for Nuclei. *Atomkernenergie* 37, 143144 (1981)

Feenberg, E.: Semi-Empirical Theory of the Nuclear Energy Surface *Rev. Mod. Phys.* 19, 239-258 (1947)

Garai, J.: The structure of the nucleus, Yearly Progress Report, Dept. of Geosciences, SUNY at Stony Brook, New York (1999)

- Garai, J.: The double tetrahedron structure of the nucleus, Physics Archive, arXiv:nucl-th/0309035 (2003)
- Garai, J.: Upper bound on the disordered density of sphere packing and the Kepler Conjecture arXiv:1001.1714v1 [cond-mat.mtrl.sci, cond-mat.dis-nn] (2010)
- Goldman, T., Maltman, K.R., Stephenson Jr., G.J., Schmidt, K.E.: The importance of nucleon substructure in nuclear ground states. Nuclear Phys. 481, 621-667 (1988)
- Hafstad, L.R., Teller, E.: The Alpha-Particle Model of the Nucleus, Physical Review, vol. 54, Issue 9, pp. 681-692 (1938)
- Haxel, O., Hans, J., Jensen, D., Suess, H.E.: on the “Magic Numbers” in Nuclear Structure. Phys. Rev. 75, 1766 (1949)
- Hofstadter, R.: The electron-scattering method and its application to the structure of nuclei and nucleons  
Nobel Lecture, December 11 (1961)
- Kienzler, B., and Geckeis, H., Radioactive wastes and disposal options, The European Physical Journal of Conferences 189, 00014 (2018)
- Lezuó, K.J.: A nuclear model based upon the close-packing of spheres. Atomkernenergie 23, 285 (1974)
- Maltman, M., Stephenson Jr., G.J., Goldman, T.: A relativistic quark model of the nuclear substructure in the  $A = 3$  system. Phys. Lett. B 324, 1-4 (1994)
- Matsui, T., Otofujii, T., Sakai, K., Yasuno, M.: Possible Structures of Pion Condensate in Symmetric Nuclear Matter Prog. Theor. Phys. 63, 1665-1687 (1980)
- Mayer, M.G.: On Closed Shells in Nuclei. II. Phys. Rev. 75, 1969-1970 (1949)
- Mayer, M.G., Jensen, J.H.D.: Elementary Theory of Nuclear Shell Structure Wiley, New York, (1955)
- Pauling, L.: The Close-Packed-Spheron Theory and Nuclear Fission. Science 150, 297-305 (1965/a)
- Pauling, L.: Structural Basis of Neutron and Proton Magic Numbers in Atomic Nuclei. Nature 208, 174 (1965/b).
- Pauling, L.: The Close-Packed-Spheron Model of Atomic Nuclei and its Relationship to the Shell model, Proc. Natl. Acad. Sci. 54, 989-994 (1965/c)
- Pauling, L.: Structural Significance of the Principal Quantum Number of Nucleonic Orbital Wave Functions Phys. Rev. Lett. 15, 499 (1965/d)
- Rainwater, J.: Nuclear Energy Level Argument for a Spheroidal Nuclear Model”. Phys. Rev. 79, 432 (1950)
- Robson, D.: Many-body interactions from quark exchanges and the tetrahedral crystal structure of nuclei Nuclear Phys. A , 308, 381-428 (1978)
- Schery, S.D., Lind, S.D., Zafiratos, C.D.: Evidence for near equality of neutron and proton radii in the  $N = 82$  isotones. Phys. Lett. B 97, 25-28 (1980)
- Wigner, E.: On the Consequences of the Symmetry of the Nuclear Hamiltonian on the Spectroscopy of Nuclei. Physical Review 51, 106-119 (1937)
- Zohuri, B., Fission Product Buildup and Decay: in Neutronic Analysis for Nuclear Reactor Systems, Springer, Cham (2019) [https://doi.org/10.1007/978-3-030-04906-5\\_15](https://doi.org/10.1007/978-3-030-04906-5_15)

## 4. Mathematical Description of the Periodic Table\*

Double tetrahedron shape with alternately arranged protons and neutrons in face-centered cubic lattice has been proposed for the structure of the nucleus (Garai, 2003). This structure reproduces the symmetry of the periodic system with no discrepancy. The structure is developed from a core tetrahedron (four nucleons) by expanding with one extra layer on both sides at each period. The number of charges in the outer shell and the nucleus are identical with the periodicity of the elements in the periodic system (Fig. 4.1). The number of lattice positions in the tetrahedron, which corresponds to the number of nuclear charge/s of the elements, should describe the sequences of the periodic table. An attempt is made here to derive analytical solutions for periodic patterns expressed by the periodic table of the chemical elements.

Analyzing the sequences of the periodic table, three repeated pattern can be identified. These patterns are named as:

fundamental [m(n)] {1, 2, 2, 3, 3, 4, 4...};

periodic [ $\Delta Z(n)$ ] {2, 8, 8, 18, 18, 32, 32...}, and;

atomic number [Z(n)] {2, 10, 18, 36, 54, 86, 118 ...} sequences,

where n is the number of period in the periodic table (Fig. 4.1).

Calculating the number of lattice positions occupied by the protons in the double tetrahedron nucleus model should reproduces all the three sequences of the periodic table.

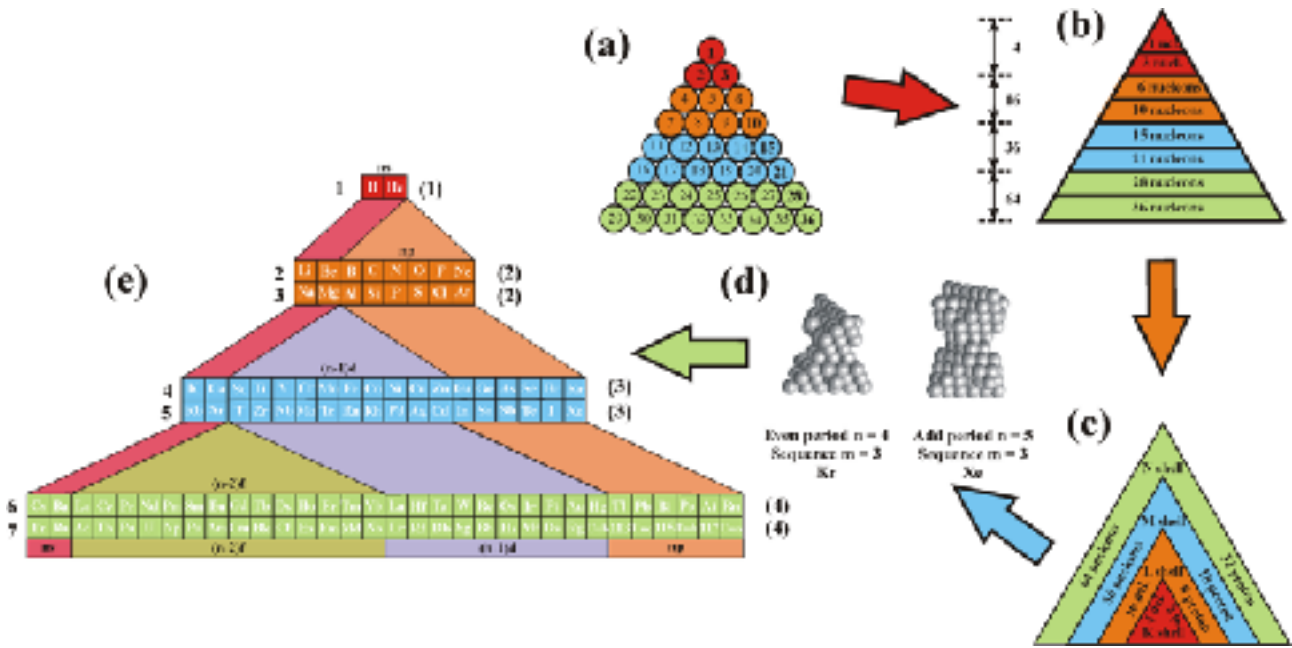
### 4.1 Fundamental Sequence

The fundamental sequence of the table expresses that each period of the table, with the exception of the first one, is repeated twice. This sequence is consistent with the proposed double tetrahedron nuclear lattice model, which, following the initial for nucleons tetrahedra, builds up its layers in two tetrahedron rotated by 90 degrees from each other (Fig. 4.1/d).

The relationship between the periods of the table (n) and the fundamental sequence numbers (m) can be described mathematically as:

$$m = \frac{2n + (-1)^n + 3}{4} \quad (4.1)$$

This expression (Eq. 4.1) reproduces the fundamental {1, 2, 2, 3, 3, 4, 4...} sequence of the periodic table.



**Figure 4.1.** The sequences of the periodic table, and the nucleons number in the double tetrahedron nuclear lattice are shown.

- (a) the number of nucleons in a triangle plane
- (b) building a face centered cubic tetrahedral lattice by stacking the triangular layers
- (c) the number of alternately arranged protons and neutrons in the outer shell of the fully developed tetrahedrons reproduces the periods of the periodic table of the elements
- (d) the 3D images of completed double tetrahedron structures for even (Kr) and for odd (Xe) periods are shown
- (e) the double tetrahedron nuclear lattice reproduces all the sequences of quantum mechanics and the periodic table

## 4.2 Periodic Sequence

Based on the proposed nuclear lattice model, the periodic sequence represents the number of protons in the two outer layers of the tetrahedron in each period. The number of lattice position in one layer can be calculated by the triangular number [Tr(k)] (Abramowitz & Stegun, 1964; Beiler, 1964). Thus, the number of nucleons in the  $k^{\text{th}}$  layer of a tetrahedron (Fig. 4.1/a) is then:

$$Tr(k) = \frac{k}{2}(k + 1) \quad (4.2)$$

In each structural development steps of the nucleus, which represents one period of the periodic table, the tetrahedron is expanded by two consecutive triangular layers on the two outer sides (Fig. 4.1/c). The number of nucleons in the outer shell of the tetrahedron [Tr(n)] is the sum of the two consecutive triangular numbers (Fig. 4.1) as:

$$Tr(n=1) = Tr(k=1) + Tr(k=2), \text{ and}$$

$$\text{Tr}(n=2) = \text{Tr}(k=3) + \text{Tr}(k=4), \text{ and so on } \dots \quad (4.3)$$

This relationship can be generalized as:

$$\text{Tr}(n) = \text{Tr}(k=2n-1) + \text{Tr}(k=2n) \dots \quad (4.4)$$

The double tetrahedron formation of the nucleus repeats the structural development of the tetrahedron twice, with the exception of the first period. Counting the same tetrahedron layers twice can be achieved by replacing the number of periods (n) with the fundamental sequence number (m). The number of nucleons in the outer shell of the double tetrahedron lattice in a given period then can be counted as:

$$\text{Tr}(n) = \text{Tr}[2m(n)-1] + \text{Tr}[2m(n)]. \quad (4.5)$$

Substituting Eq. 4.2 into Eq. 4.5 gives the nucleon numbers in the outer shell of the tetrahedron in each periods as:

$$\text{Tr}(n) = 4[m(n)]^2 \quad (4.6)$$

The number of protons in a given layer is half of the total available lattice positions. Thus, the number of charges  $[\Delta Z(n)]$  in the completely developed layers of the tetrahedron is

$$\Delta Z(n) = \frac{\text{Tr}(n)}{2} = 2[m(n)]^2 \quad (4.7)$$

Substituting the sequence number (m) from Eq. 4.1 gives the formula for the periodic sequence as:

$$\Delta Z(n) = \frac{1}{8}[2n + (-1)^n + 3]^2 \quad (4.8)$$

The formula for the periodic sequence (Eq. 4.8) had been identified, and derived by previous studies (Tomkeieff, 1951; 1954). This is the only mathematical expression of the three presented sequences of the periodic table, which had been derived by previous studies.

### 4.3. Atomic Number Sequence

The expression, giving the total number of charges in the nucleus with completely developed shells, can be derived in a similar manner. The total number of nucleons in a tetrahedron with k layers can be determined by its tetrahedral number  $[\text{Th}(k)]$  (Abramowitz & Stegun, 1964; Conway, 1996)

$$\text{Th}(k) = \frac{k}{6}(k + 1)(k + 2) \quad (4.9)$$

It can be seen from Eq. 4.5 the layers of the tetrahedron corresponds to the fundamental sequence number (m) as:  $k=2m$ , where m is the function of the periods (n) as given in Eq. 4.1.

The number of lattice sites in one completed tetrahedron, given as the function of the fundamental sequence number (m), can be written then as:

$$Th(m) = \frac{m}{3}(2m + 1)(2m + 2) = \frac{4m^3}{3} + 2m^2 + \frac{2m}{3} \quad (4.10)$$

The double tetrahedron nucleus is alternately expanded two tetrahedrons, which is rotated by 90 degrees. The number of lattice sites in the double tetrahedron ( $Th^{double}$ ) in odd number periods are twice as the two tetrahedron numbers minus 4, because the first period is a single one. The total number of lattice sites for odd number of periods is then:

$$Th^{double}(n^{odd}) = 2Th[m(n)] - 4 \quad (4.11)$$

In even periods, only one of the tetrahedron is completed. This can be taken into account by deducting the number of lattice sites which has not been developed. The number of lattice sites in the  $n^{th}$  period [ $Tr(n)$ ] in the outer layers of the tetrahedron can be calculated by Eq. 4.6.. The number of nucleons in the double tetrahedron in even periods is then

$$Th^{double}(n^{even}) = 2Th[m(n^{even})] - Tr[m(n^{even})] - 4. \quad (4.12)$$

The formula

$$\frac{(-1)^n + 1}{2} \quad (4.13)$$

can be used to generate 0 for odd periods and 1 for even number periods. The general solution for both odd and even periods is then

$$Th^{double}(n) = 2Th[m(n)] - \frac{(-1)^n + 1}{2} Tr[m(n)] - 4 \quad (4.14)$$

The number of charges in the nucleus in a completely developed sequence ( $Z(n)$ ) is half of the available lattice positions. Therefore,

$$Z(n) = \frac{Th^{double}(n)}{2}. \quad (4.15)$$

Combining Eqs. (4.1), (4.6), (4.9), (4.14) and (4.15) gives the number of nuclear charges for any period. The atomic number sequence of the periodic table can be described then as:

$$Z(n) = \frac{1}{3}[4m^3 - [(-1)^n - 1]3m^2 + 2m - 6] \quad (4.16)$$

Substituting m from Eq. (4.1) gives the atomic number sequence as:

$$Z(n) = \frac{1}{48}[2n + (-1)^n + 3]^3 - \frac{1}{16}[(-1)^n - 1][2n + (-1)^n + 3]^2 + \frac{1}{6}[2n + (-1)^n + 3] - 2$$

(4.17)

Any physical models proposed for the explanation of PSCE have to explain and reproduce the sequences of the periodic table. The proposed double tetrahedron nuclear lattice model complies with this condition.

The sequence of the Principle Quantum Numbers [PQN(n)] is given as:

$$S_{PQN} = \{ 2, 8, 18, 32 \dots \} \quad (4.18)$$

The first two entries are the same in both the sequence of the principal quantum number and the sequence of the length of the period. The rest of the entries in these sequences show similarity but they are not identical. The sequence of the principal quantum number can be given as:

$$PQN(n) = 2n^2 \quad (4.19)$$

This formula [Eq. (4.19)] emerging from quantum theory does not agree with any of the sequences of the periodic table [Eqs.(4.1, 4.8, 4.17)] indicating that quantum mechanics cannot give a viable explanation for the sequences of the periodic table.

#### 4.4 Conclusions

The symmetry pattern of the periodic system of the chemical elements emerges from the nuclear charge. This invariant pattern can be maintained only if the positions of the nucleons are also invariant. Thus the nucleons should form a lattice structure. The lattice arrangement of the nucleons is consistent with the Pauli exclusion principle and offers a feasible physical explanation for the exclusion principle. Representing protons and neutrons with equal spheres, arranging them alternately in an FCC lattice, and developing a tetrahedron, rotating by 90 degrees at each expansion, results in an identical symmetry pattern expressed by the PSCE.

Based on the presented nuclear lattice model, mathematical solutions for the sequences of the periodic table are derived. Investigating the structural development of the nucleus it is shown that the periodicity of the electronic structure is the natural outcome of the nuclear lattice geometry. The presented tetrahedron lattice model is the first nucleus model which is able to reproduce all of the sequences of the periodic table. It offers a credible physical explanation for the identical symmetry of the nucleus and the electronic structure, for the Pauli exclusion principle and for the Aufbau principle.

The one by one agreement between the sequences of the periodic table of the chemical elements and the double tetrahedron nuclear lattice eliminates the likelihood of possible coincidence. This indicates that the double tetrahedron nuclear lattice model should be considered as a reliable physical explanation for the organizing principles of the periodic table of the chemical elements.

## References to Chapter 4

This chapter was published in the International Journal of Quantum Chemistry in 2008.

\* Garai, J., Mathematical Formulas Describing the Sequences of the Periodic Table, *International Journal of Quantum Chemistry*, 108, 667-670 (2008)

Abramowitz, M.; Stegun, I.A. Handbook of Mathematical Functions; National Bureau of Standards Applied Math. Series 1964, 55, 828.

Beiler, A.H. Recreations in the Theory of Numbers; Dover, NY, 1964, p. 189.

Conway, J.H.; Guy, R.K. The Book of Numbers; Copernicus Press, NY, 1996, p. 83.

Garai, J. Physics Archive, 2003, arXiv:nucl-th/0309035v2

Tomkeieff, M.V. Nature 1951, 167, 954.

Tomkeieff, M.V. Nature 1954, 173, 393

## 5. Electronegativity of the elements\*

Electronegativity is one of the most important concepts in chemistry and measures the affinity of the atoms for electrons in a compound. Jöns Jacob Berzelius (Jensen, 1996) initiated the idea in 1811, and Linus Pauling gave a quantitative description in 1932. Pauling suggested that the energy of the polar covalent bond comes from two sources - from purely covalent bond energy and from the energy emerging from partial ionic attraction. The partial ionic contribution to the bond energy was described with the square of the difference of the electronegativities of the two elements as:

$$c \left| \chi_A - \chi_B \right|^2 = D_o(AB) - \frac{D_o(AA) + D_o(BB)}{2} \quad (5.1)$$

where  $D_o(AA)$ , and  $D_o(BB)$  are the dissociation energies of A-A and B-B bonds, and  $D_o(AB)$  is the dissociation energy of an A-B bond,  $\chi_A$ , and  $\chi_B$  are the electronegativities of the two elements, and  $c$  is a scaling factor. Currently the geometric mean is used instead of the arithmetic one. Giving the dissociation energies of the bonds in  $KJmol^{-1}$  the bond energy can be calculated as:

$$D_o(AB) = \sqrt{D_o(AA) D_o(BB)} + 96.3(\chi_A - \chi_B)^2 \quad (5.2)$$

Pauling assigned the value of 4 for the electronegativity of fluorine and calculated all the other values from the experimentally defined bond dissociation energies. Investigating Pauling's bond energy–bond polarity description, it was found that the Pauling scale works well for bonds with low polarity (Murphy, 2000). In the past decades, other alternative descriptions of electronegativity have been proposed.

Robert Mulliken (1934;1935) suggested to calculate electronegativity ( $\chi_M$ ) as the average of the ionization energy (I), and the electron affinity, ( $E_{ea}$ ) as:

$$\chi_M = \frac{|I + E_{ea}|}{2} \quad (5.3)$$

This relationship suggests that both ionization energy and electron affinity linearly increase electronegativity. High ionization energy indicates that the atom would not release electrons readily, and the high electron affinity indicates that it is energetically favorable to acquire electrons. Both of these assumptions make physical sense. Empirical formulas, how to convert the Mulliken ( $\chi_M$ ), and the Pauling ( $\chi_P$ ) electronegativities from one to the other, had also been suggested (David & Heric, 2005).

Allred and Rochow (1958) defined electronegativity ( $\chi_{AR}$ ) as the electrostatic force exerted by the nucleus on the valence electrons as:

$$F = \frac{Z^*e^2}{4\pi\epsilon_0r_c^2} \quad (5.4)$$

where  $Z^*$  is the effective nuclear charge, either measured experimentally, or calculated using Slater's rule,  $e$  is the charge of the electron,  $\epsilon_0$  is the permittivity of free space and  $r_c$  is the covalent radius. Using a scaling factors to line up with Pauling values the Allred-Rochow electronegativity can be calculated as:

$$\chi_{AR} = 0.359\frac{Z^*}{r_c^2} + 0.744, \quad (5.5)$$

where the covalent radius is in Angstroms. Ghosh et al. (2009) suggested that the absolute (most probable) and not the covalent radii should be used when the electronegativity of the atoms is evaluated.

The “spectroscopic” or Allen (1989; 1994; 2000) electronegativity ( $\chi_{spec}$ ) is described by the average one-electron energy of the valence shell electrons, which can be calculated as:

$$\chi_{spec} = \frac{m\epsilon_s + n\epsilon_p}{m + n} \quad (5.6)$$

where  $\epsilon_s$ , and  $\epsilon_p$  are the ionization energies of the s and p electrons, and m and n are the numbers of electrons in the s and p shells respectively.

Rahm and Hoffman (2018) recently proposed electronegativity should be calculated from the average valence binding energy at ground state as:

$$\chi = \frac{\sum_{i=1}^n n_i\epsilon_i}{n} \quad (5.7)$$

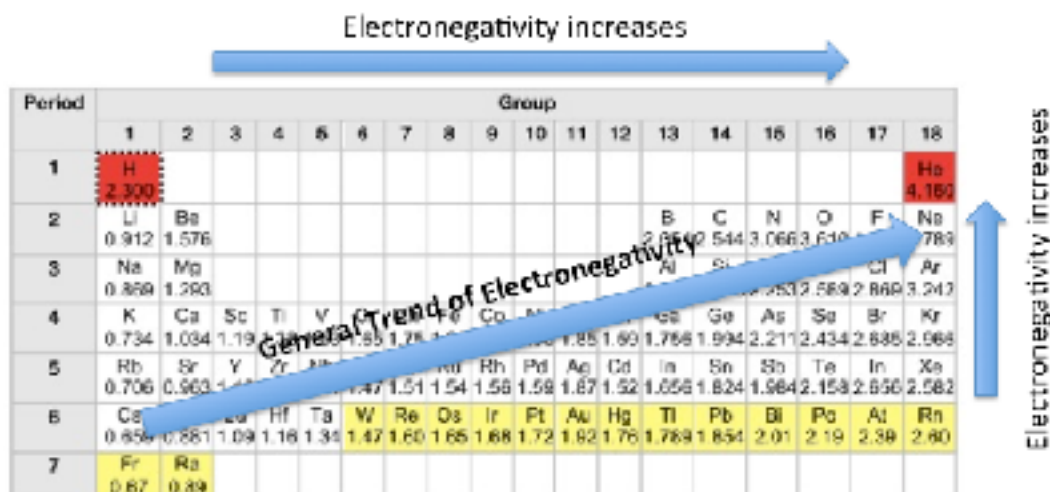
where  $\epsilon_i$  is the energy of the  $i^{\text{th}}$  shell  $n_i$  is the occupation of the  $i^{\text{th}}$  level, and n is the total number of electrons.

With conversion factors, all of these alternatives are approximately in line with each other and with the original Pauling scale.

The currently used semi empirical relationships calculate electronegativity from different physical parameters, which indicate that there is no consensus on the theoretical base of electronegativity.

## 5.1 Electronegativity pattern of the elements

Electronegativity of the elements is periodic, and follows a regular trend organized by the periodic table (Fig. 5.1). This trend is sometimes called the third dimension of the periodic table (Murphy et. al, 2000). In the groups of the periodic table, electronegativity decreases with the atomic number, while in the periods it increases. This regular trend shows irregularity in the first period and for elements with higher atomic number than 74 (W).



**Figure 5.1** The electronegativity of the elements (Allen, 1989, 1994), and the general trend is shown in the periodic table. Elements with irregular electronegativity are highlighted.

The pattern of electronegativity, which is governed by the periodic table, indicates that the organizing principle behind electronegativity should be the same as for the periodic table.

It is discussed in chapter 3 and 4 that the periodicity of the chemical elements originates from the nuclear lattice. The relevant characteristics of the nuclear lattice model to electronegativity are briefly discussed here.

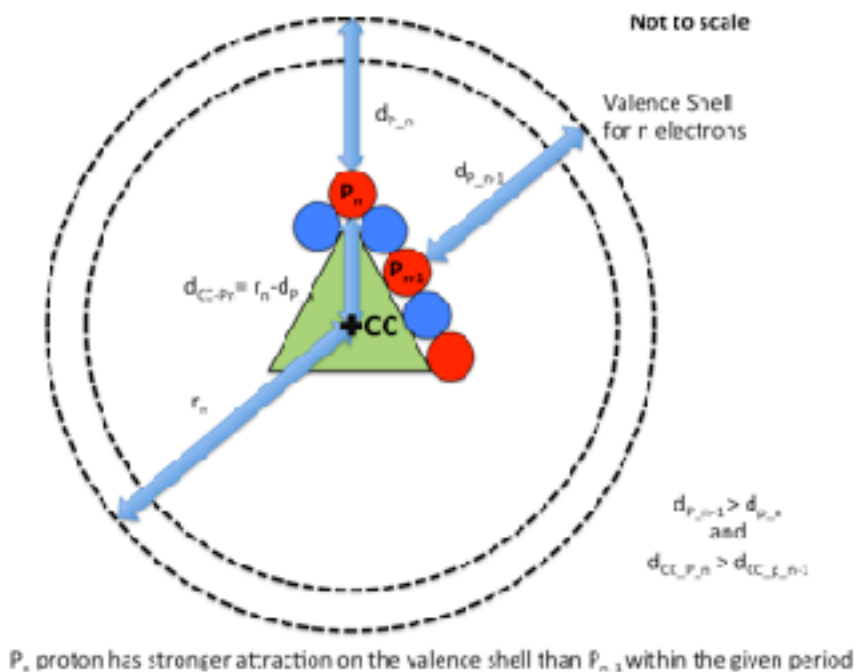
## 5.2 Nuclear lattice model

The point charge representation of the nuclear charge is oversimplified. Protons and neutrons are individual particles occupying certain space in the nucleus. The best candidates describing the nucleon arrangements in the nucleus are the nuclear lattice models (Pauling, 1965/a, b, c, d; Cook, 2010; Garai, 2018).

These models assume that protons and neutrons have the same size and they are arranged in the closest packing lattice. Closest packing arrangements built up from tetrahedron and octahedron units of the equal spheres. Expanding the nucleus from a tetrahedron unit reproduces the periodicity of the periodic table (Garai, 2008). The images of the completely developed structures, the last elements in the periodic table, is shown on Figure 3.5.

One of the important outcomes of the nuclear lattice models is that each and every proton has its well-defined lattice position, which is consistent with the Pauli exclusion principle. The electrostatic attractions of the positive charges on the valence electron shell depends on the distance between the individual protons and the electron shell. The distance between the charge center of the nucleus and the newly added proton of an element ( $d_{CC-p}$ ) increases within the period as the protons and neutrons build up the outer layers of the tetrahedron nuclear lattice (Fig. 5.2). Thus, as the period developing, the last added proton of the given element gets closer and

closer to the valence electron shell. Consequently, the attraction of the protons on the valence shell becomes stronger and stronger. How the distances are changing between the valence electron shell and the individual protons, in relation to the periodic table, is discussed in the next chapter.



**Figure 5.2** The schematic figure of the positions of the protons and neutrons in the nucleus and their distance from the valence shell is shown. The protons are red, the neutrons are blue, and  $CC_n$  is the charge center of the nucleus. Please note that the charge center of the nucleus changes when an additional proton is added. The strength of the attractions is the smallest at the beginning of the period (one proton) and getting stronger as the period develops because the distance between the newly added proton and valence electron shell decreases.

The different distance between the individual protons and the valence electron shell results in a different attraction of the protons on the valence shell. It is suggested that this attraction is the physical explanation behind electronegativity. The increasing electronegativity in a period is consistent with this proposed physical explanation. The exceptions or irregularities of this general trend are discussed in paragraph 5.4.

### 5.3 Activation of electronegativity

The calculated average valence energy, and consequently electronegativity, is the highest for the elements in group 18<sup>th</sup>. The average proton-valence shell distance ( $d_{i-average}$ ) is also the smallest for the noble gasses in each period. Despite their highest electronegativity, the chemical characteristic of these elements is inert, with no affinity to electrons at all. This characteristic of the noble gasses emerging from the definition of electronegativity, which can only be interpreted in relation to covalent bond (Pauling, 1932; 1960). Thus, electronegativity is “activated” at the formation of the covalent bond. Noble gasses have the highest average valence electron energy or electronegativity; however, this electronegativity is “latent” because it is not

activated. This condition, electronegativity needs to be activated in covalent bonds, is not included in the original Pauling description of electronegativity (Eq. 5.2). The dissociation energy of a compound is calculated by adding the covalent and ionic contributions of the bond energies. Based on this relationship noble gases should have ionic bond contribution and react with other elements, with lower electronegativity. This is contradict with experiments. It is suggested that in order to generalize equation 5.2, including the noble gasses, the following condition should be added. If either of the dissociation energies of AA, or BB is zero, then the energy of AB must be zero too. Thus, the bond energy should be defined as:

$$D_o(AB) = \sqrt{D_o(AA) D_o(BB)} + 96.3(\chi_A - \chi_B)^2$$

$$\text{if } D_o(AA) D_o(BB) = 0, \text{ then } D_o(AB) = 0 \quad (5.8)$$

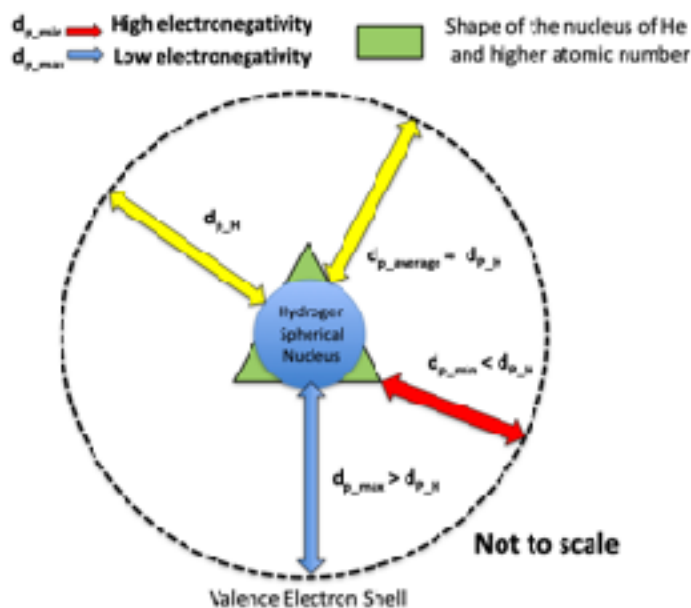
Please note that Eq. 5.8 does not take into account the London dispersion, which is always active and can bond the atoms together.

## 5.4 Irregularities

It is discussed in chapter 2.4 that in the long form of periodic table, based on the definition of groups, Hydrogen can be placed as alkali metal or as a halogen. From the outermost electronic configuration point of view, Hydrogen has one  $1s^1$  electron; therefore it should be placed in the first group. However, it needs only one electron to attain inert configuration; therefore, it can also be placed in the 17th (halogen) group. Given that, chemically hydrogen behaves both as a halogen as well as alkali metal, the position of Hydrogen is still uncertain (Scerri, 2007; Laing, 2007) in the periodic table. The position of Helium in the periodic table is also contradictory. The outermost configuration of Helium is  $1s^2$ , therefore, it should belong to the second column. However; the chemical properties of Helium are equivalent to inert gases. Based on the chemical properties, the position of Helium is in group 18 in the long form of the periodic table. Note that, all the other elements in the 18th group have  $ns^2 np^6$  electronic configuration in their valence shell. The electronegativity of Hydrogen and Helium are not consistent with their electronic structure.

### 5.4.1 Electronegativity of Hydrogen

The nuclear structure of Hydrogen contains one proton. Thus, the shape of the nucleus of the Hydrogen is spherical. Distributing charges on the surface of a sphere and a tetrahedron, which has the same volume, is shown on Figure 5.3. The distance of the charges to the valence shell is shown for the two different nuclear shapes. Thus, the average distance of the charge/s on a spherical nucleus could be equivalent to a tetrahedron nucleus around the middle of the period. This conclusion can be justified easily by the visual inspection of the nuclear shapes (Fig. 5.3).



**Figure 5.3** It can be seen by visual inspection, the average distance between the valence electron shell and the charge on the surface of a spherical nucleus is constant. This distance in a tetrahedron nuclear lattice is continuously decreasing within the period. If the volume and the proton number are equal for a sphere and a tetrahedron nucleus then the average distance of the charges from the valence electron shell would be equal around the middle of the period for the two nuclear shapes. Since the average distance corresponds to electronegativity, the electronegativity of Hydrogen should be the same as the elements situated in the middle of the period. This theoretical conclusion is consistent with the known chemical characteristics of Hydrogen.

The same average distance between the nuclear charge and the valence shell corresponds to the same electronegativity. Thus, electronegativity of a nucleus with a spherical shape in relation to the tetrahedron should be equal when about half of the tetrahedron outer layer of the nuclear lattice is filled, which is in the middle of the period. Thus, the right place for Hydrogen in the periodic table should be in column 14. Helium with its completed tetrahedron nuclear structure should be in-group 18, which is the current position of He in the contemporary periodic table. The deduced positions from nuclear structure of the elements in the first period are supported by and consistent with the chemical characteristics of these elements.

#### 5.4.2 Electronegativity of Tungsten and beyond

The other irregularity in the electronegativity pattern occurs for the elements with higher atomic number than 74 (W). These elements do not decrease but rather increase electronegativity as the atomic number increases in the group. This “feature” of the regular trend of electronegativity is also the consequence of the tetrahedron lattice structure of the nucleus. The presented explanation is quite speculative, but makes common sense, and consistent with the double tetrahedron nuclear model.

Neutrons and protons are arranged alternately in the nuclear lattice of the elements. There is no need for additional neutron/s for bonding the protons in the first three periods of elements. Beyond Calcium, elements with higher atomic numbers require additional neutrons for their stability. In the double tetrahedron nucleus the periods alternately build the tetrahedron lattice. Thus the lattice sites of the six periods built on the layers of the fourth period (Fig. 5.4).



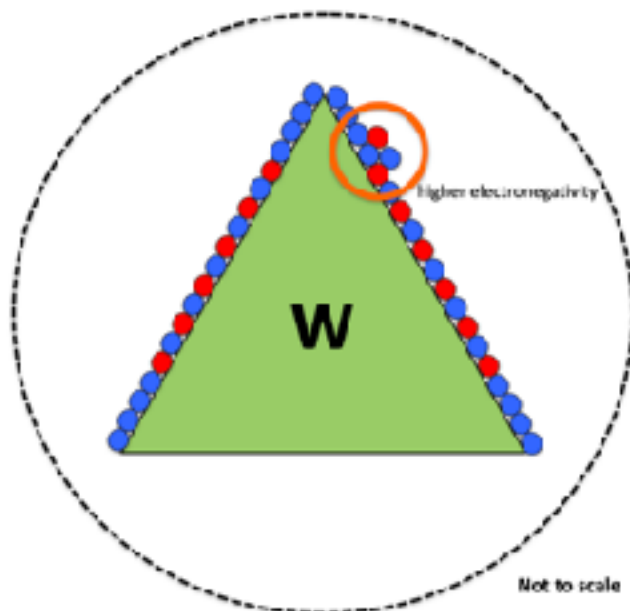
**Figure 5.4** Schematic figure of one of the tetrahedron, showing the layers for the six periods of the periodic table. For deeper insight see also Figure 3.5 in chapter 3.

The number of extra neutrons at the end of the periods are calculated by subtracting the proton number multiplied by two from the atomic weight.

4 period (Ca)	→	$40 - 2 \times 20 = 0$	extra neutrons
4 period (Kr)	→	$84 - 2 \times 36 = 12$	extra neutrons
5 period (Xe)	→	$131 - 2 \times 54 = 23$	extra neutrons
6 period			
(up to W)	→	$184 - 2 \times 74 = 36$	extra neutrons

The number of extra neutrons from period 4 is 12. The extra neutron numbers in the six periods up to tungsten is 36 minus the extra neutron numbers of period 5, which gives 13. The number of lattice sites for the alternately arranged protons and neutrons in the six periods up to tungsten is  $(74 - 54) \times 2 = 40$ . The total number of protons and neutrons in the six layers of the tetrahedron lattice is  $12 + 13 + 40 = 65$ . The total available lattice site for the entire period is 64, which is fulfilled for tungsten. Thus, the added proton for tungsten and the elements beyond that must occupy the next layer of the tetrahedron lattice (Fig. 5.5). In this case the protons are closer to the valence electron shell resulting in higher electronegativity.

The identical agreement, between the available lattice sites for the 6<sup>th</sup> period and the additional neutron number strongly supports both the double tetrahedron nuclear lattice model, and the proposed theoretical explanation for electronegativity.



**Figure 5.5** The 2D schematic figure of the nucleus of Tungsten is shown. The additional neutrons plus the protons of the elements in the six period, fulfill the available lattice positions. The only available lattice site for the added proton is in the next layer of the tetrahedron lattice, which is closer to the valence electron shell, resulting in higher electronegativity.

## References to Chapter 5

This chapter was presented at The 28<sup>th</sup> annual Conference of The International Society for the Philosophy of Chemistry (ISPC 2025).

\*Garai, J., Nuclear Lattice Model Offers Physical Explanation for Electronegativity, The 28<sup>th</sup> annual Conference of The International Society for the Philosophy of Chemistry (ISPC 2025), Antwerp, July 9-11 (2025)

Allen, L. C. Electronegativity is the average one-electron energy of the valence-shell electrons in ground-state free atoms *J. Am. Chem. Soc.* **1989**, 111, 9003-9014.

Allen, L.C., Chemistry and Electronegativity, *Int. J. Quantum Chemistry*, **1994**, 49, 253-277.

Allred, A.L., Rochow, E.G. A scale of electronegativity based on electrostatic force. *J. Inorganic Nuclear Chemistry*. **1958**, 5, 264-268.

Cook, N.D. *Models of the Atomic Nucleus*, 2nd ed. Springer, Berlin. ed. (2010).

David R. Herrick, D.R. Connecting Pauling and Mulliken Electronegativities. *Journal of Chemical Theory and Computation* 2005, 1 (2), 255-260. DOI: 10.1021/ct049942a

Garai, J. Nuclear lattice model and the electronic configuration of the chemical elements, in *Mendeleev to Oganesson. A Multidisciplinary Perspective on the Periodic Table*, Edited by Eric Scerri and Guillermo Restrepo, Oxford University Press (2018)

Garai, J. Mathematical formulas describing the sequences of the periodic table. *Int. J. Quant. Chem.*, **2008**, 108, 667-670.

Ghosh, D.C, A new scale of electronegativity based on absolute radii of atoms *J. Theor. Comp. Chem.* **2005** 4(1) 21-33.

- Ghosh, D.C., Chakraborty, T., and Mandal, B., The electronegativity scale of Allred and Rochow: revisited, *Theor Chem Acc*, **2009**, 124: 295-301.
- Jensen, W.B. Electronegativity from Avogadro to Pauling: Part 1: Origins of the Electronegativity Concept. *J. Chem Ed.* **1996**, 73, 11-20.
- Laing, M., Where to put Hydrogen in a periodic table? *Foundations of Chemistry*, **2007**, 9(2) 127-137.
- Mann, J.B., Meek, T. L., Allen, L. C. Configuration Energies of the Main Group Elements. *J. Am. Chem. Soc.* **2000**, 122, 2780-2783.
- Mulliken, R. S. A New Electro affinity Scale; Together with Data on Valence States and on Valence Ionization Potentials and Electron Affinities". *Journal of Chemical Physics* **1934**, 2, 782–793.
- Mulliken, R. S. Electronic Structures of Molecules. XI. Electroaffinity, Molecular Orbitals and Dipole Moments. *J. Chem. Phys.* **1935**, 3, 573-585.
- Murphy, L.R., Meek, T.L., Allred, A.L., Allen, L.C. Evaluation and Test of Pauling's Electronegativity Scale, *J. Phys. Chem. A* **2000**, 104, 24, 5867-5871.
- Pauling, L. The Nature of the Chemical Bond. IV. The Energy of Single Bonds and the Relative Electronegativity of Atoms. *J. Am. Chem. Soc.* **1932**, 54, 3570-3582.
- Pauling, L. *The nature of the chemical bond*, Cornell University Press, Ithaca, New York (1960) ; pp. 64-97.
- Pauling, L. The close-packed-spheron theory and nuclear fission. *Science*, **1965**, 150, 297–305.
- Pauling, L. Structural basis of neutron and proton magic numbers in atomic nuclei. *Nature*, **1965**, 208, 174.
- Pauling, L. The close-packed-spheron model of atomic nuclei and its relationship to the shell model. *Proc. Natl. Acad. Sci.* **1965**, 54, 989–994.
- Pauling, L. Structural significance of the principal quantum number of nucleonic orbital wave functions. *Phys. Rev. Lett.*, **1965**, 15, 499.
- Rahm, M., Hoffmann, R. Electronegativity Seen as the Ground State Average Valence Electron Binding Energy. *J. Am. Chem. Soc.* **2018**, 141, 10.1021/jacs.8b10246.
- Sanderson, R.T. Electronegativity and Bond Energy. *J. Am. Chem. Soc.* **1983**, 105(8) 2259-2261.
- Scerri, E.R., *The periodic table – its story and significance*, New York, Oxford University Press (2007)

## 6. Electronic Structure of the Atoms

The most important sequence in the development of the electronic structure of the chemical elements is the {2, 8, 8, 18, 18, 32, 32...} pattern which represents the number of elements in each period of the periodic table or the number of electrons in each completed shell. The periodicity pattern for the ground state neutral atoms and for the positive atomic ions is different (Brakel, 2000; Goudsmith & Richards, 1964). The simplest manifestation of periodicity, the ground state neutral atoms, are investigated here.

The interaction between the proton and electron is the result of the exchange of virtual photons. Based on the energies of the electrons in the atoms, virtual photon or quantum electrodynamic treatment is not necessary when the classical approach is sufficient to describe the interaction. In this study classical electromagnetism approach is used to answer how protons in the nuclear lattice can control the electronic structure of the elements.

One of the outcomes of the nuclear lattice model is that the nucleus cannot be considered as a point charge. The lattice position of a given proton must be taken into consideration when the attraction on an electron shell is calculated. The relative attractive force  $[F_{e-p}(Z)]$  of a proton  $[P(Z)]$  on an electron  $[e(Z)]$  can be characterized by the distance between the charge center of the nucleus and the proton  $[d_{NCC(Z)-P(Z)}]$ .

$$F_{e-p}(Z) = f(d_{NCC(Z)-P(Z)}). \quad (6.1)$$

where  $Z$  is the corresponding atomic number defined as follows: The first proton in the Hydrogen nucleus is  $P(1)$ , the next proton added into the structure to form the nucleus of Helium is  $P(2)$  and the last proton added to the nuclear structure of element  $Z$  is  $P(Z)$ . The electrons are labeled accordingly. Thus electron (1) is captured by  $P(1)$  and electron ( $Z$ ) is captured by  $P(Z)$ . Please note that the position of the charge center changes, when an additional proton is added to the nucleus. The charge center relating to proton number  $Z$  is given in subscript as:  $NCC(Z)-P(Z)$ .

Depending on the lattice positions of proton ( $Z$ ) the attraction can be either stronger or weaker than the attraction of proton ( $Z-1$ ). The relative attraction of proton  $Z$  and  $Z+1$  can be defined by comparing the distances between the charge center of the nucleus to the positions of these two protons as:

$$d_{P-NCC(Z+1)}(Z) < d_{P-NCC(Z+1)}(Z+1) \quad \text{then} \quad F_{P-e}(Z) < F_{P-e}(Z+1) \quad (6.2)$$

or vice versa (Fig. 6.1). The closer position of a proton to the nuclear charge center relates to weaker attraction on the valence electron shell.

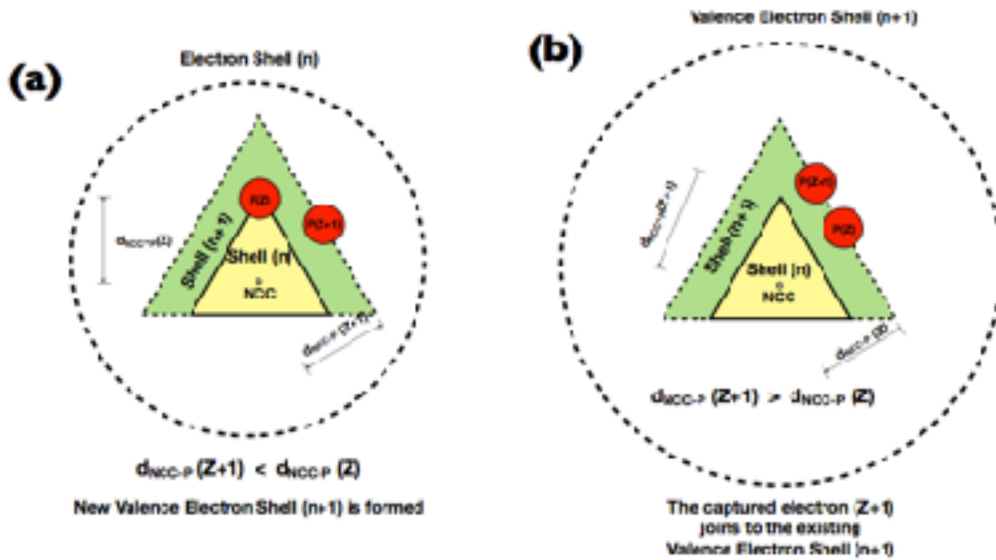
In order to overcome the repulsive force of the existing electrons in the valence shell, the relative attractive force on the newly captured electron ( $Z+1$ ) must be stronger than the relative attraction force on the electrons already occupying the valence shell. This requires to comply with the following inequality:

$$F_{P-e}(Z+1) > F_{P-e}(Z) \quad \Leftrightarrow \quad d_{P-NCC(Z+1)}(Z+1) > d_{P-NCC(Z+1)}(Z). \quad (6.3)$$

This inequality is consistent with the Aufbau principle, which states that orbitals with the lowest energy are filled first. When this condition (Eq. 6.3) is not satisfied then it is predicted that the electron is unable to join to the valence shell and starts to form a new valence shell outside of the existing one (Fig. 6.1/a). Thus, a new electron shell should start to form when

$$F_{P-e}(Z+1) < F_{P-e}(Z) \Leftrightarrow d_{P-NCC}(Z+1) < d_{P-NCC}(Z) \quad (6.4)$$

Based on stability considerations the first proton in the new nuclear shell should be positioned at the middle of the new layer of the tetrahedron and this new outer layer of the structure should develop towards the edges. It can be seen by visual inspection that in a given nuclear shell equation 6.3 or the Aufbau principle is satisfied (Fig. 6.1/ b) until the completion of the given layer of the nuclear structure.



**Figure 6.1.** Schematic figure in 2D showing the geometry of the nucleus.

(a) If the distance of the proton (Z+1) in a new nuclear layer is closer to the nuclear charge center than the distance of the proton (Z), completing the previous shell, then a new electron shell is formed, since the captured (Z+1) electron is unable to overcome the repulsion of the existing electron shell (Eq. 6.4).

(b) The distance between the nuclear charge center (NCC) and the proton increases as the protons occupy the lattice positions in the same layer from the middle to the edge of the tetrahedron resulting in stronger attraction on the captured electrons (Eq. 6.3). Thus, the electrons can join to the existing valence shell until the completion of the nuclear structure, which is the end of the period.

The distance of the last proton completing a shell [n] and the distance of the first proton in the new shell [n+1] is calculated from the nuclear charge center. It is assumed that the position of the last proton in layer n is at the vertex of the tetrahedron and the position of the first proton in layer n+1 is at the surface, closest to the charge center (Fig. 6.1/a). It is also assumed that the charge center of the nucleus coincides with the mass center. For the completed structures of the tetrahedron He, Ne and “double” tetrahedron Ar, Xe and Ra nucleus, the mass center coincides with the charge centers. When a new nuclear shell is started by adding a

proton, then the charge center shifts towards the proton, resulting in a smaller distance between the charge center and the proton than the distance between the proton and the mass center. Thus using the mass center instead of the charge center is a conservative estimate on the inequality of  $d_{P-NCC(Z+1)}(Z+1) < d_{P-NCC(Z+1)}(Z)$ .

The distance between the first proton in the shell and the mass center is calculated first. For simplification the length of the edge of the basic tetrahedron is one unit. Thus the diameter of the nucleons is also one unit. The height of a tetrahedron [ $h_{\Delta}$ ] with unit length is

$$h_{\Delta} = \sqrt{\frac{2}{3}}. \quad (6.5)$$

Assuming a unit mass for the nucleons the distance between the vertex of the tetrahedron and the mass center is:

$$d_{\Delta\text{vertex-MC}} = \frac{3}{4}h_{\Delta} = \sqrt{\frac{3}{8}} \quad (6.6)$$

The distance between the face of the tetrahedron and the mass center is then:

$$d_{\Delta\text{surface-MC}} = \frac{1}{4}h_{\Delta} = \sqrt{\frac{1}{24}} \quad (6.7)$$

The tetrahedron is expanded by one-one layers on both sides; thus the length of the side of the tetrahedron is increased by two units in each of the periods (Fig. 6.1). The distance between the center of a sphere (nucleon lattice position), placed on the surface of the tetrahedron, and the mass center in period  $n+1$  is then

$$d_{\Delta\text{surface-MC}}(n+1) = (2n+1) \frac{1}{4}h_{\Delta} = (2n+1) \sqrt{\frac{1}{24}} \quad (6.8)$$

where  $n$  is the number of the period. The distance between a sphere placed at the vertex of the tetrahedron in period  $n$  can be calculated then as:

$$d_{\Delta\text{vertex-MC}}(n) = (2n-1) \frac{3}{4}h_{\Delta} = (2n-1) \sqrt{\frac{3}{8}} \quad (6.9)$$

It can be seen that

$$d_{\Delta\text{vertex-MC}}(n) > d_{\Delta\text{surface-MC}}(n+1) \quad (6.10)$$

where  $n = 2, 3, 4, 5, \dots$  Arranging the nucleons in an FCC lattice and building up a tetrahedron, the inequality in equation 6.4 is fulfilled when a new layer in the nuclear structure starts to form (Fig. 6.1/a). Thus

$$\begin{aligned} & d_{P-NCC}(Z=2) > d_{P-NCC}(Z=3) \quad \bullet \quad d_{P-NCC}(Z=10) > d_{P-NCC}(Z=11) \quad \bullet \quad d_{P-NCC}(Z=18) > d_{P-NCC}(Z=19) \\ & \bullet \quad d_{P-NCC}(Z=36) > d_{P-NCC}(Z=37) \quad \bullet \quad d_{P-NCC}(Z=54) > d_{P-NCC}(Z=55) \quad \bullet \quad d_{P-NCC}(Z=86) > d_{P-NCC}(Z=87). \end{aligned} \quad (6.11)$$

The remaining rest of the pairs of the elements ( $[Z] \Leftrightarrow [Z+1]$ ) satisfy the relationship of equation 6.3 and  $[d_{p-NCC(Z+1)}(Z+1) > d_{p-NCC(Z+1)}(Z)]$ . Thus, the captured new electrons for these elements can join to the existing valence electron shell (Fig. 6.1/b).

As a result of the inequalities of Eq. 6.11, the relative attractive force on the newly captured electron is weaker than the force on the electrons in the existing shell, leading to the formation of a new electron shell for the following elements:

$$F_{p-e}(\text{He}) > F_{p-e}(\text{Li}) \quad \bullet \quad F_{p-e}(\text{Ne}) > F_{p-e}(\text{Na}) \quad \bullet \quad F_{p-e}(\text{Ar}) > F_{p-e}(\text{K}) \\ F_{p-e}(\text{Kr}) > F_{p-e}(\text{Rb}) \quad \bullet \quad F_{p-e}(\text{Xe}) > F_{p-e}(\text{Cs}) \quad \bullet \quad F_{p-e}(\text{Rn}) > F_{p-e}(\text{Fr}) \quad (6.12)$$

Based on the presented geometrical consideration, it is suggested that the cyclical structural development of the nuclear structure results in an interruption of the development of valence shells because the relative attraction of the proton on the captured electron becomes weaker when a new layer starts to built in the nucleus (Garai, 2011). The cycles of the weaker relative attractions predicted from the geometry of the nuclear structure are identical to the length of the periods in the periodic table. It is concluded that the electronic configuration of the chemical elements is the consequence of the structural development of the nuclear lattice.

## References to Chapter 6

This chapter was published in the book Mendeleev to Oganesson. A Multidisciplinary Perspective on the Periodic Table in 2018.

\*Garai, J., Nuclear lattice model and the electronic configuration of the chemical elements, in Mendeleev to Oganesson. A Multidisciplinary Perspective on the Periodic Table, Edited by Eric Scerri and Guillermo Restrepo, Oxford University Press (2018)

Brakel van, J.: Philosophy of Chemistry. Leuven University Press. Leuven, Belgium. (2000)

Garai, J.: Physical Model Explaining the Periodic Pattern of the Chemical Elements. arXiv:1101.4478v1[physics.gen-ph] (2011)

Goudsmith, S.A., Richards, P.I.: The order of electron shells in ionized atoms, Proc. Natl. Acad. Sci. USA **51**, 664–671 (1964)

## 7. The Stability of the Opposite Charges in the Atoms\*

The atoms contain oppositely charged particles, protons and electrons. These particles are stable in the atoms and do not annihilate each other. The stability of these opposite charges can be ensured by static or dynamic equilibrium.

Based on Earnshaw's theorem two equal but opposite charges can only be in stable stationary equilibrium, if at least one of them is not a point but a distributed charge. The free electron is a point charge. Thus, the static equilibrium of the opposite charges would require distributed positive charge in the atom. Based on this theoretical conclusion Thomson proposed a "plum pudding" model for the structure of the atoms. The scattering experiments of Hans Geiger and Ernest Marsden, supervised by Rutherford, showed that there is a small, but heavy positively charged core (nucleus) inside the atom, which consist almost the entire mass of the atom. Thus, these experiments indicate that both the electron/s and the nucleus should be considered as point charges. These point charges can be stable only if the attraction of the nucleus on the negatively charged electron/s is balanced out by the centrifugal force of the orbiting electron/s.

The dynamic equilibrium of the opposite charges in the atom has many shortcomings. Based on electromagnetism; the accelerating charged particle should emit radiation. This energy loss would spiral the electron into the nucleus. Atoms are stable in the timescale of the universe and in ground state no radiation is emitted. In order to eliminate this discrepancy, between the stability of the atoms and classical electromagnetism, Bohr postulated that parts of the laws of electromagnetism are not valid at atomic scale. This statement has never been supported by any theoretical explanation. Bohr's postulate not only lacks theoretical justification but more importantly contradicts with experiments. Decelerating electrons near the nucleus do emit radiation (Bremsstrahlung), indicating that the laws of classical electromagnetism remain valid at atomic scale. Consequently, the non-emitting electrons in the atoms should have stationary position.

The opposite charges in the atoms are in equilibrium. Experiments showed that both the electron and the nucleus can be considered as point charges. Thus, the possibility of static equilibrium should be excluded.

However, there is one important difference between the experiments detected point charge nature for both the electron and the nucleus. The point charge nature of the nucleus had been verified in the atom, while the point charge nature of the electron had been concluded from the investigation of free, non-bonded electrons\*\*. The point charge nature of the captured electron in the atom has never been verified experimentally. It is investigated that are the free and bonded electrons identical or these electrons might differ from each other?

### 7.1 Characteristics of the free and bonded electrons

Investigating the characteristic features of the free and bonded electrons it can be seen that these electrons are not identical but rather differ from each other. The noticeable differences between the free and bonded electrons are listed here.

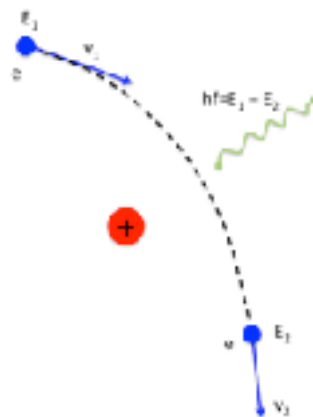
**7.1.1** Electrons are assumed to be identical, indistinguishable particles, with no internal structure. Electrons are defined as fermions, which obey the Pauli exclusion

principle, and follow the Fermi-Dirac statistics. The Fermi-Dirac statistic is defined as:

$$f(E) = \frac{1}{Ae^{\frac{E - E_F}{kT}} + 1} \quad (7.1)$$

where  $f(E)$  is the Fermi function, expressing the probability at thermal equilibrium, that an available state at energy  $E$  will be occupied by an electron,  $E_F$  is the Fermi energy,  $k$  is the Boltzmann constant, and  $T$  is the absolute temperature. The  $+1$  is the consequence of the Pauli exclusion principle, it guarantees that  $f(E) \leq 1$ . The Fermi-Dirac statistic describes the occupancy of the energy levels by electrons in solids. Thus, this description refers to bonded electrons in an atom, and it is not applicable to free electrons.

**7.1.2** Bonded orbiting electrons in the atoms do not emit radiation. Decelerating free electrons when they deflected by an atomic nucleus do emit electromagnetic radiation, which is known as Bremsstrahlung (Figure 7.1). The lack of emission of the electrons in the atoms indicates that these electrons should be in static equilibrium with the nucleus.



**Figure 7.1** The electron decelerates in the vicinity of an opposite charge, emitting a Bremsstrahlung radiation. No emission of the neutral atoms is observed, which contradicts with the point charge orbiting electron model.

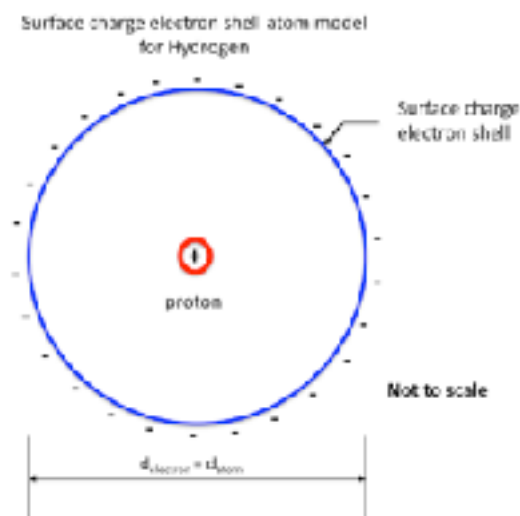
**7.1.4** Bounded electrons in the atom do not interact with the magnetic field contrarily to free electrons. The non-interaction of the bonded electrons with the magnetic field is also an indicator of static equilibrium between the nucleus and the electron/s.

**7.1.5** The law of electromagnetism applies to free but not to bound electrons. There is no theoretical basis why the laws of electromagnetism partially cease to exist in the vicinity of the nucleus and are not applicable to bonded electrons. If the validity of classical electromagnetism at atomic scale is accepted then this is a clear indicator of static electron/s in the atom.

**7.1.6** Bounded electrons have spin (Gerlach & Stern 1922). This spin is not detectable for free electrons. Niels Bohr propagated the idea that the magnetic

moment of the free electron could not be observed. However, this suggestion is not supported by experiments (Garraway & Stenholm 2002).

The list of the different behavior of the free and bonded electrons might not be complete but it should be convincing enough from the listed differences, the free and bonded electrons are not identical. The different behavior of the free and bonded electrons can be resolved if the electron in the atom is in static equilibrium with the nucleus. This equilibrium requires that the point charge electron must be transferred to surface charge. It is suggested that the point charge free electron transfers to surface charge when captured by the nucleus, and that the electrons form a spherical surface charge around the nucleus (Garai, 2017). The proposed atom model for Hydrogen is shown on Figure 7.2.



**Figure 7.2** Schematic figure of the Hydrogen atom is shown. The two opposite charges remain stable only if the point charge electron transforms to a spherical surface charge around the nucleus.

In the next chapter it is investigated how this “phase transformation” of the electron, from point to surface charge at capturing, and vice versa, fits to and consistent with the characteristic features of the atoms.

## References to Chapter 7

This chapter was published in Physics Essays in 2017.

\* Garai, J., The electronic structures of the atoms, Physics Essays, 30(4), 455-460 (2017)

and presented at PSA around the world II, with a focus on Eastern and Central Europe in 2025,

\*Garai, J., The stability of the opposite charges in the atoms, Book of Abstracts, PSA around the world II, with a focus on Eastern and Central Europe, 79-81, November 6, 14 and 22 (2025)

\*\*Based on the standard definition, the electron is free, when the potential field is zero. In this text the expression of free electrons refers to non-bonded electrons.

Garraway, B.M.; Stenholm, S. (2002) Does the Flying Electron Spin? *Contemporary Physics*, 43, 3, 147-160.

Gerlach, W.; Stern, O. (1922) Der experimentelle Nachweis der Richtungsquantelung im Magnetfeld  
*Zeitschrift Physik*, 9, 349-352.

## **8. Non-revolving Surface Charge Electron Shell Model\***

The different features of the atoms are described by quantum mechanics. It has been stated in chapter 1 after almost a hundred years there is still no consensus in the scientific community why this mathematical treatment is able to correctly describe the characteristic features of the electron. How the proposed surface charge electron shell model fits to the quantum mechanical description is discussed first.

### **8.1 Quantum mechanics**

Quantum mechanics offers the currently available best description of the atoms. It assumes that all phenomena at atomic scale can be described by the wave function.

The fundamental problem with Bohr's planetary model was that the orbiting point charge electron is a one-dimensional model; therefore, it is only able to reproduce the main quantum numbers. Schrödinger (1926) wave equation describes the behavior of the electron in three-dimension. Different descriptions of the wave function had been proposed by Dirac, which is physically identical with Schrödinger's wave equation, and differs only in the mathematical formalism. This purely mathematical approach is able to reproduce all the known features of the Hydrogen atom.

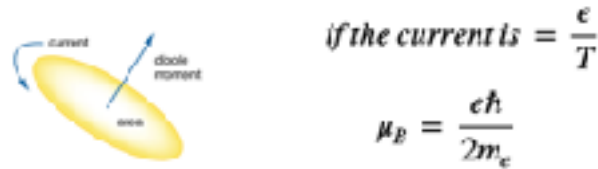
If the electron would be a point charge, then one variable, the radius, would be enough to describe the vibration of the electron. This is certainly insufficient; therefore, the captured electron in the atom must be three dimensional, as assumed by Schrödinger's wave equation, which describes the vibration of a spherical surface in three-dimension. The three spatial quantum numbers relate to the spherical harmonics of the vibrating shell. The fourth quantum number relates to the spin of the electron. The quantum mechanical description of the spin depicts the direction of a randomly propagating wave in the surface charge electron shell, which is also consistent with the model.

It is suggested that the surface charge electron shell model of the atoms offers a viable physical explanation for the quantum mechanical treatment of the electrons.

### **8.2 The main emission lines of the Hydrogen atom**

Disturbing the equilibrium of the non-revolving surface charge electron shell induces ripples on its surface. These ripples propagate as waves in the surface charge electron shell. The calculated velocity of the propagating wave in the surface charge electron shell for the Hydrogen atom is identical with the Bohr's velocity (Garai, 2017). The propagating waves in the surface charge electron shell; therefore, reproduces the main emission lines of the Hydrogen atom. It also reproduces the value of the Bohr's magneton (Fig. 8.1).

## Bohr's magneton



**Figure 8.1** Schematic figure of the Bohr's magneton in the Hydrogen atom. The propagating wave in the surface charge electron shell of the atom can generate the same magnetic moment as an orbiting point charge electron.

### 8.3 Zero angular momentum of the Hydrogen atom at ground state

The angular momentum of the Hydrogen atom at ground state is zero ( $L = 0$ ). The Bohr model contradicts with this feature of the Hydrogen atom, because it predicts  $L = \hbar$  instead of zero.

At ground state there is no wave propagation in the surface of the electron shell because of the lack of “disturbance”. This is consistent with the experimentally verified ground state zero angular momentum.

### 8.4 Single valued condition of the Schrödinger wave-equation

The boundary condition of Schrödinger's wave function is that the variable must return to its initial value. In one dimension, the condition, can be stated as:

$$\Psi(x) = \Psi(x + nL), \text{ where } n = \pm 0, 1, 2, 3... \quad (8.1)$$

where  $\Psi(x)$  is the wave function, and  $L$  is the length of the wavelength. The outcome of the single valued description of the wave function is that the angular momentum must be quantized.

The wave description of a point charge electron does not require to comply with the single valued condition. However, the vibration of a continuum, like a spherical surface charge, must satisfy this condition.

### 8.5. Quantized nature of the angular momentum

Based on the size constraint of the shell the length of the propagating wave must be quantized, resulting from the single valued constraint. The angular momentum of this propagating wave can be described as:  $L_n = n\hbar$ , where  $\hbar$  is the reduced Planck constant. The wavelengths of the propagating waves are the harmonics of the vibrating spherical valence electron shell. The quantized nature of the angular momentum requires a continuum charge distribution.

### 8.6 No emission in stationary states

It is an experimental fact that no emission occurs at stationary states. This requires complete destructive interference of the vibrating electron/s. It is impossible for a

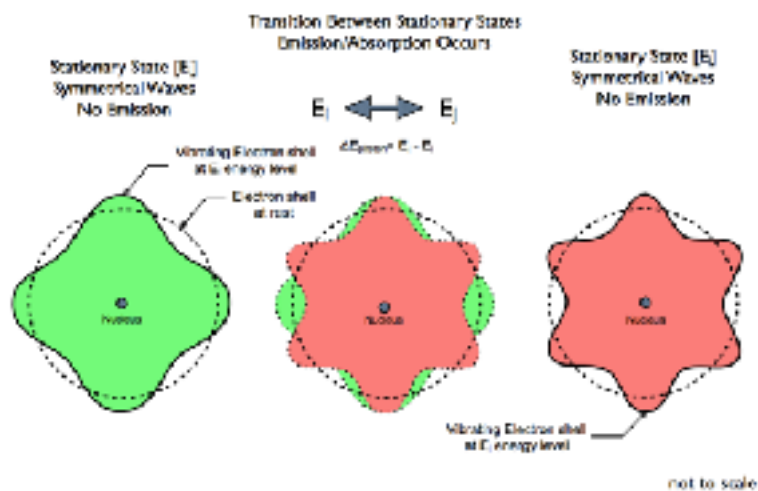
single point charge electron to destructively interfere with itself, like in the Hydrogen atom.

The stationary vibration of the surface charge electron shell is symmetrical and completely destructive, with no emission.

### 8.7 Photon emission and absorption

Photons are only emitted or absorbed in an atom when transition occurs between the stationary vibration states of the electron. It has been discussed that the stationary waves in the surface charge electron shell vibrate symmetrically. The induced electric and magnetic fields of the vibration are interfering destructively; therefore, as long as the frequency of the standing wave remains the same no emission occurs.

When the vibration switches from one symmetrical mode (stationary state) to another one, then during the transition period, the vibration becomes asymmetric, resulting in a photon emission. In reverse, photon absorption can transfer the energy to the vibrating shell triggering a transition between the stationary states (Fig. 8.2).



**Figure 8.2** Schematic 2D figure shows the occurrence of the emission and the absorption of the electromagnetic radiation at atomic scale. The vibration of the electron halo around the nucleus is symmetrical at the stationary energy levels. Thus, no emission occurs resulting from destructive interference. However, when the transition occurs between one symmetrical vibration state to another symmetric one then the asymmetric vibration during this transition period results in emission or absorption of electromagnetic radiation. The uniform surface charge distribution of the electron offers a physical explanation for the emission and absorption of photons without violating the laws of classical electromagnetism.

### 8.8 The electron shells of the atoms can transfer force or stress

The transfer of force from one atom to another one is impossible if the opposite charges are in dynamic equilibrium, since the stability of the orbiting electron/s would be destabilized.

The surface charge electron shell of the atoms is a continuum; therefore, capable of carrying and transferring force or stresses without violating the stability of the opposite charges in the atoms.

### 8.9 The long-term stability of the atoms

The orbit of a point charge electron around the nucleus in the time scale of the universe should be chaotic. Even the solar system, with enormous orbiting bodies,

and relatively long orbiting frequency, is chaotic in a hundred million and longer time scales. Consequently, the dynamic equilibrium of the opposite charges in the atom can not be maintained because after certain time would become chaotic. Thus, in the time scale of the universe, none or very few stable atoms should exist.

The long time stability of the atoms can only be guaranteed by non-orbiting static surface charge electron shell/s of the atoms.

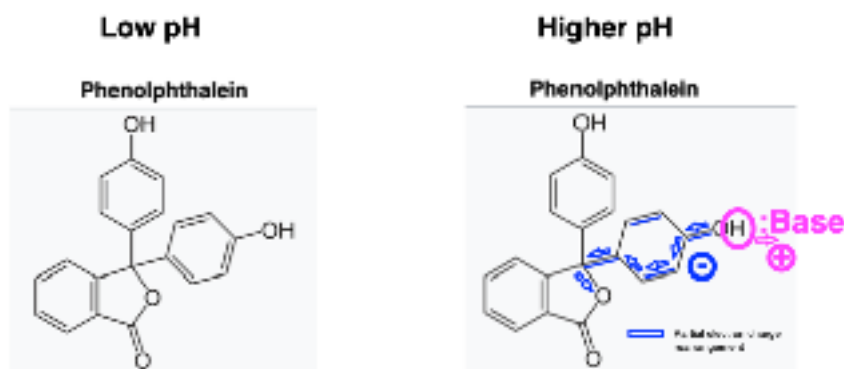
### 8.10 Polarizability of the atoms

It is well known from chemistry; electric charge is capable of changing its distribution in an atom. This non-uniform charge distribution, and the capability of the redistribution of the charge of the electrons in the atoms or molecules, is well demonstrated by the following features: dipole, induced dipole, dipole induced dipole and London dispersion forces. This non-uniform charge distribution, and the capability of the redistribution of the charge of the electrons in the atoms cannot be explained by unit point charges which are in dynamic equilibrium in the atom.

Partial distribution of the charge in the atom is only possible, if the charge of the electron/s in the atoms is distributed charge. Thus, polarizability requires continuum charge distribution.

### 8.11 Partial charge rearrangement in molecule

If the surrounding electric field changes around a molecule then the molecule can compensate for this effect by rearranging its charge. One example might be the phenolphthalein in different pH environments (Fig. 8.3)



**Figure 8.3** Partial electron charge rearrangement is shown in Phenolphthalein in low and high pH.

This kind of fractional unit charge rearrangement is possible only if the electron is not a unit point charge but distributed one.

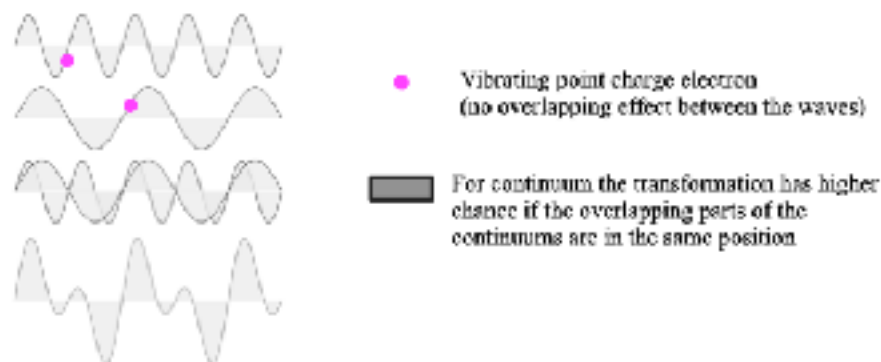
### 8.12 Transition intensity

The spontaneous transition intensity of the spectra depends on the overlapping of the wave equations of the vibrating states. It can be calculated as:

$$\left| \int_{r=0}^{r=+\infty} \psi_{n_i} \psi_{n_f} dr \right|^2 \propto \text{spontaneous transition intensity} \quad (8.2)$$

where  $\psi_{n_i}$  and  $\psi_{n_f}$  are the wave functions for the initial and final states respectively.

The overlapping of the vibration can only be effective if the vibrating charge is a continuum (Fig. 8.4).



**Figure 8.4** The overlapping effect on the spontaneous transition intensity for vibrating point charge and continuum.

The proposed phase transformation of the electrons not only explains the stability of the opposite charges but is also consistent with quantum mechanics and all the known features of the atoms. The theoretical consistency with experiments should qualify the surface charge electron shell atom model, to be considered as a viable alternative describing the structure of the atoms.

## References to Chapter 8

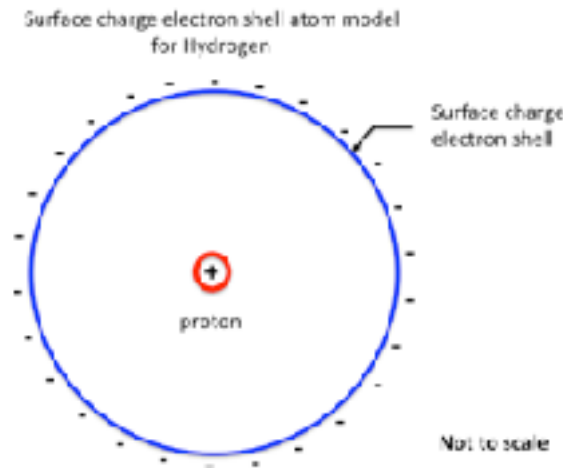
This chapter was published:

- \*Garai, J., The electronic structures of the atoms, *Physics Essays*, 30 (4) 455-460 (2017)
- \*Garai, J., A Paradigm Shift in Physics and Lattice Confinement Fusion, *Infinite Energy*, 164, 28-29 (2023)
- \*Garai, J., Atomic Structure: Validation of the Electron Phase Transformation Theory. *Chemical Science International Journal* 32 (6):78-89. (2023)
- \*Garai, J., Examining the Electron Phase Transformation Theory in the Context of Atomic Structure, *Chemical Science International Journal* 33 (4):11-18 (2024)

## 9. Phase Transformation of the Electron\*

If the phase transformation of the electron from point to surface charge is valid then almost all the energy of the charge formation should be released as the charge expands from point to the atomic surface size, and vice versa. This energy increase is not observed in the atoms when an electron is captured. It is possible that the energy of the charge formation of the electrons is transferred and stored in the atom in a different form. This possibility is investigated.

It has been concluded that classical electromagnetism is valid at atomic scale (Garai, 2017; 2023). Assuming that the charge of the proton is uniformly distributed on its surface then the non-revolving static spherical electron shell around the proton can be considered as a spherical capacitor (Fig. 9.1).



**Figure 9.1** The schematic figure of the Hydrogen atom is shown. The proton and the non-revolving, static, surface charge electron shell around the nucleus can be considered as a spherical capacitor. The stored energy of this capacitor agrees reasonably well with the rest energy of the electron. The energy balance indicates that the formation of an atomic capacitor is a feasible physical process to explain the energy transfer of the electron at the phase transformation.

Capacitors store energy. The energy balance of the phase transformation of the electron would require that the energy stored by the atomic capacitor should be almost the same as the rest energy of the electron. The charge formation energy of the surface charge electron shell is minor, since the radius of the shell is the Bohr's radius. This energy is neglected in the calculations. The energy equivalency of the phase transformation of the electron is investigated for the simplest atomic structure, the Hydrogen atom.

Based on Maxwell's equations the capacitance of the Hydrogen atom ( $C_H$ ) can be calculated as:

$$C_H = \frac{4\pi\epsilon_0 a_0 r_p}{a_0 - r_p} = 9.36199 \times 10^{-26} F \quad (9.1)$$

where  $\epsilon_o$  is the vacuum permittivity,  $a_o$  is the Bohr's radius, and  $r_p$  is the radius of the proton. The energy stored on this "atomic capacitor" of the Hydrogen atom ( $E_{H-Cap}$ ) is

$$E_{H-Cap} = \frac{1}{2} \frac{q_e^2}{C_H} = 1.37095 \times 10^{-13} \text{ J} = 8.55682 \times 10^5 \text{ eV} \quad (9.2)$$

where  $q_e$  is the charge of the elementary charge. The stored energy in the capacitor of the Hydrogen atom is slightly higher than the rest energy of the electron:

$$E_{H-Cap} > m_e c^2, \quad (9.3)$$

where  $m_e$  is the mass of the electron, and  $c$  is the speed of light in vacuum. In equations 9.1-9.3, the recommended values of CODATA (NIST 2018) are used for the physical constants.

Assuming energy balance between the rest energy of the electron and the formed atomic capacitor gives the following equality:

$$\frac{q_e^2(a_o - r_{P-atom})}{8\pi\epsilon_o a_o r_{P-atom}} = m_e c^2 + \frac{q_e^2}{4\pi\epsilon_o} \left( \frac{1}{r_P} - \frac{1}{r_{P-atom}} \right) \quad (9.4)$$

where  $r_{P-atom}$  is the radius of the proton inside the Hydrogen atom. The added term to equations 9.1-9.3 in equation 9.4 represents the energy resulting from the modified size of the proton in the atom. Manipulating the equation and expressing the proton radius inside the Hydrogen atom gives the proton size in the Hydrogen atom as:

$$r_{P-atom} = \frac{3q_e^2}{8\pi\epsilon_o m_e c^2 + 2q_e^2 \frac{a_o + r_P}{a_o r_P}} = 9.718907 \times 10^{-16} \text{ m} \quad (9.5)$$

This proton radius is about 15 percent bigger than the current consensus, recommended by CODATA (NIST 2018). The proton radius is measured for individual protons. In the Hydrogen atom the proton is surrounded by an attracting negative surface charge. It is possible this attraction slightly increases the size of the proton in the atom.

The energy equivalence between the formed atomic capacitor and the rest energy of the electron in the Hydrogen atom indicates that the phase transformation of the electron from point to surface charge and visa versa is energetically feasible. The energy of the charge formation of the electrons is stored in the formed capacitor in the atom.

## References to Chapter 9

This chapter was published in Physics Essays in 2024.

\*Garai, J., (2024) The phase transformation of the electron forms an atomic capacitor, Physics Essays 37, 3, 200-201.

Garai, J., (2017) The electronic structures of the atoms, Physics Essays, 30 (4) 455-460; DOI: 10.4006/0836-1398-30.4.455

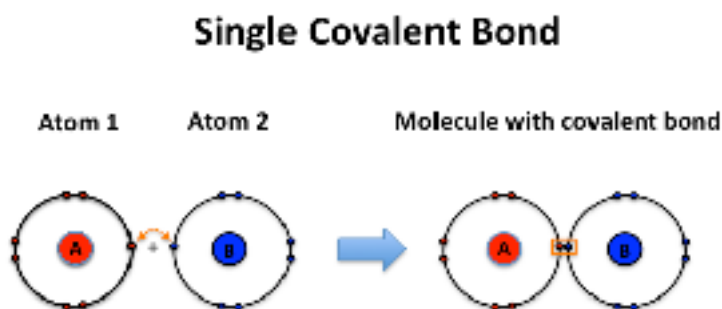
Garai, J., (2023) Atomic Structure: Validation of the Electron Phase Transformation Theory, Chemical Science International Journal, 32(6), 78-89; DOI: 10.9734/CSJI/2023/v32i6873

## 10. Electron sharing in covalent bonds\*

The empirical concept, sharing the valence electrons results in bond formation, had been deduced from experiments about a century ago. Quantum mechanics interprets the covalent bond formation as the result of the overlapping of the wave functions. The formation of covalent bonds is one of the most fundamental chemical processes. Despite its importance, there is no adequate physical explanation how and why the shared electrons, or the overlapping of the wave function could bond atoms together.

### 10.1. Introduction

The concept of chemical bonds goes back to Newton, who stated in 1704 that the atoms attract each other by some force. In 1916 based on the chemical experience of the time, Gilbert Lewis (1916) suggested that the bond formation relates to the shared electron pair/s between the atoms. The attraction of the bond is attributed to the mutual attraction of the two positively charged nuclei. The electron-sharing concept of the covalent bonds (Fig. 10.1) explains many molecular features. The concept is very useful, and widely used, even in current chemistry, despite lacking physical explanation. The history and the current understanding of the Lewis electron-sharing model are discussed in Zhao et al. (2019/a).



**Figure 10.1** Schematic figure of the Lewis interpretation of covalent bonding. The shared electrons form electron pairs between the atoms. The energy of these bonding pairs results from the simultaneously attracted two atomic nuclei. This model explains many features of covalent bonding but lacking physical explanation, and has many shortcomings.

Quantum mechanics assumes that the bond is the consequence of the interference of the atomic wave functions (Heitler & London 1927). The description of the orbiting electron is probabilistic. In the case of more than one electron, since the electrons are interacting with each other, it is impossible to calculate reliably the overall probabilities of the electrons. In order to overcome this problem, the calculations of bond energies employ simplifying assumptions. The most popular theoretical approaches, describing the bonds, are the Valence Bond, the Molecular Orbital and the Density Functional theories (Zhao et al. 2019/b). Despite all the progress that has been made in our understanding of covalent bonds in the past century there is no consensus on the physical interpretation of the bonds (Weisberg 2008; Needham 2014; Nordholm & Bacskay 2020; Scerri 2023). Even the existence of the bond in reality is questioned (Seifert 2023). Eric Scerri (2022) concluded his plenary talk at ISPC, 2022 “Perhaps philosophers of chemistry should attend to this genuine debate in understanding the nature of chemical bonding instead of withdrawing into metaphysical questions such as whether bonds exist or whether they are real”. Covalent bonds are undoubtedly exist, eventhough, physical explanation for the bonds is lacking.

Based on the reinterpretation of previous experiments, a non-revolving surface charge electron shell atomic structure had been proposed in chapters 7-9. In the enlightenment of this new electronic structure, the known physical characteristics of the covalent bonds are collected and analyzed.

## 10.2 Characteristic features of covalent bonds

Covalent bonds exhibit characteristic physical features, which are deduced from experiments. These features are the following.

### 10.2.1 Overlapping of the orbitals

According to quantum mechanics the overlapping of the electron orbitals results in covalent bond formations. The orbital electron density of the **s** electrons is spherical, while the orbital of the **p** electrons is dumbbell shaped. Based on quantum mechanics, the overlapping of these different orbitals results in different covalent bond formations.

#### $\sigma$ bonds

If the atomic orbitals have cylindrical symmetry around the bonding axis then the formed molecular orbital is  $\sigma$ , or the name of the formed bond is  $\sigma$  bond. The electron density, in this case, is concentrated between the two nuclei of the bonded atoms. There is no node in the overlapping electron orbitals (Fig. 10.2). Generally, all single bonds are  $\sigma$  bonds formed by **s-s** orbitals. It is also possible to form  $\sigma$  bonds from overlapping of **s-p** or **p-p** atomic orbitals.

#### $\pi$ bonds

The side-by-side overlapping of the electron orbitals results in  $\pi$  bonds. The higher electron density of the bond is concentrated on the two sides of the inter nuclei axis of the bond, which results in a lateral overlap of the orbitals. Thus, there is a node between the overlapping **p** orbitals, which are forming  $\pi$  bonds (Fig. 10.2).



**Figure 10.2** Schematic figure of the overlapping of the electron clouds is shown in 2D for  $\sigma$  and  $\pi$  bonds.

### 10.2.2 Order of bond formation

Covalent bonds can be formed by one electron pair (single bond) or more than one electron pair (double or triple bonds). The single bonds are always  $\sigma$  bonds. The double covalent bond contains one  $\sigma$  and one  $\pi$  bond, while the triple covalent bond contains one  $\sigma$  and two  $\pi$  bonds. Thus, multiple bonds require  $\sigma$  and  $\pi$  bonds, where  $\sigma$  bonds are always formed first.

### 10.2.3 Saturation of the bond

Ionic bonds are non-saturated, the electrostatic attraction is active outside of the bonded atoms, and have omni-directional electrostatic interaction between the positively and negatively charged ions. Covalent bonds are saturated, containing only the bonded atoms. There is no electrostatic attraction outside of the bonds, and covalent bonds are directional, where the regions of different electron densities bind atoms together along particular trajectories (Weisberg 2008). Thus, molecules with pure covalent bonds are neutral, with no electrostatic attraction outside of the bonded atoms.

### 10.2.4 Valence Shell Electron Pair Repulsion (VSEPR)

Electrons with the same charges repel each other. The higher electron densities in covalent bond along with the lone pairs of the molecules are moderately destabilizing. Consequently, in order to minimize the repulsive effect of these bonds and lone pairs, the distances between the bonds and lone pairs of the molecule are maximized. This improves the overall stability of the molecule. The repulsion is the strongest between two lone electron pairs, medium between bonding and lone pairs, and the lowest between two bonding electron pairs. The distances, minimizing the repulsion, can be defined from the number of bonds and lone pair electrons. These distances allow us to predict the structural arrangement of the atoms in a molecule.

### 10.2.5 Delocalization of the electrons

In certain cases the molecules can be represented by more than one equivalent Lewis structure. These structures differ only in the location of the  $\pi$  orbitals but chemically they represent the same molecule. Resonance theory states that if the molecule or ion can be represented by two or more Lewis structures, which differ only by the position of the  $\pi$  electrons then the structure should be represented as a hybrid or average of these structures. The electrons in a  $\sigma$  bond have a fixed location so they are localized. On the other hand  $\pi$  electrons can be delocalized and be in different locations. In other words, the number of the bonding  $\pi$  electrons do not necessarily integer, but a fraction of the electron pair might participate in the bonding.

Good example of resonance structure is benzene, where the carbon ring is flat and the carbon-carbon bonds have a mixed single and double bond characters. The delocalized electron pairs of the  $\pi$  bonds do not have an integer value. The measured length between the atoms is consistent with the assumed delocalization. The bond distance, between the carbon atoms in benzene, is between the bond-length of the single and the double carbon bonds (ex. Berkovitch-Yellin and Leiserowitz 1975).

### 10.2.6 Bond electron density

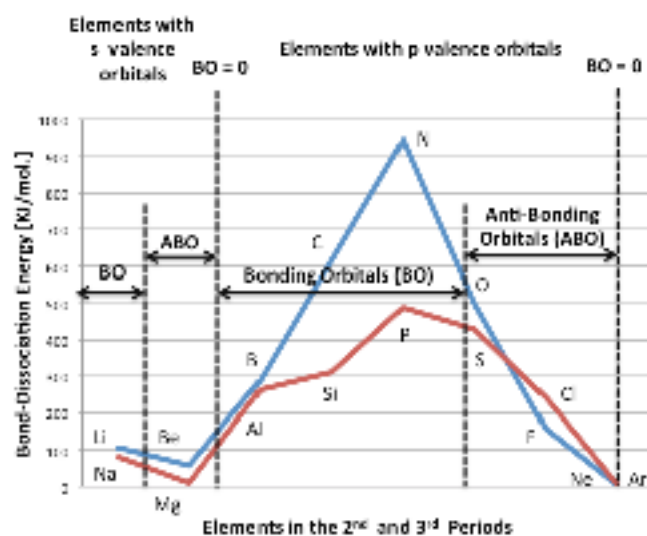
Based on x-ray diffraction the electron density of the atoms can be determined by experiments. It is well established that bonding electron pairs have higher charge densities than lone pair electrons. Knowing the positions of the atoms, the electron densities of the undistorted or not bonded single atoms can be calculated. The difference of the experimentally observed and calculated undisturbed electron density gives the deformation density of the electron shell. This deformation density correlates to the electron density of the bonds. The bond density on average is 0.1 electron/bond, which is about 5 percent of the "Lewis bond" (ex. Berkovitch-Yellin and Leiserowitz 1975; Dunitz 1983).

### 10.2.7 Potential models

The potentials of covalent bonds are described by the two classic pair potentials, the Morse and the Lennard-Jones. Both potentials consist of a short-range repulsion and a longer-range attraction with two adjustable parameters (Morse 1929; Lennard-Jones 1931). Based on these potential wells, beside the attraction of the nucleuses, the electrons in the valence shell must be repelled by the same charges in order to have a stable energy minimum of the bond.

### 10.2.8 Bond Dissociation Energy

The bond dissociation energies of neutral atoms in one period of the periodic table correlate to the atomic number or the number of unscreened protons in the nucleus. The trends for the s and the p orbitals are shown for the second and third periods of the periodic table (Fig. 10.3). This trend remains the same for higher periods. Based on current consensus, the bond dissociation energy increases with the number of the protons in the nucleus resulting from the stronger attraction. This effect is dominant as long as the bonding orbitals are not completely filled. When the bonding orbitals are filled then the dissociation energies start to decrease despite the stronger attraction of the nucleus because the anti-bonding orbitals of the molecule are filled. The dissociation energies of the elements can be calculated from the energies of the bonding and anti-bonding molecular orbitals.



**Figure 10.3** The bond-dissociation energies for the 2<sup>nd</sup> and 3<sup>rd</sup> periods of the periodic table are plotted as a function of increasing atomic number (Rumble et al. 2023). The dissociation energies of the elements in a period increase until a maximum is reached and then decrease. Higher periods exhibit a similar trend.

Currently, no physical model is known, which can comply with all the features of covalent bonding (11.2.1-8). It is investigated that how the non-revolving electron shell model fits to and comply with the features of covalent bonds.

### 10.3. Physical model for covalent bonds

The essence of covalent bonding is the electronic structure of the atoms, which is discussed in chapters 7-9. It was concluded that in order to comply with the known features of the free and the bonded electrons, and the atoms, the electron must go through phase transformation from point to surface charge when captured by the

nucleus and vice versa. The formed non-revolving surface charge electron shell model of the atoms is shown in Fig. 10.4. It is investigated how this electronic structure complies with the characteristic features of the covalent bonds.



**Figure 10.4** The schematic of the non-revolving surface charge electron shell atom model is shown. The unique feature of the model is that the electrons are not point charges but form surface charge halo around the nucleus. The nuclear lattice (Garai 2008, 2018) is represented by a triangle.

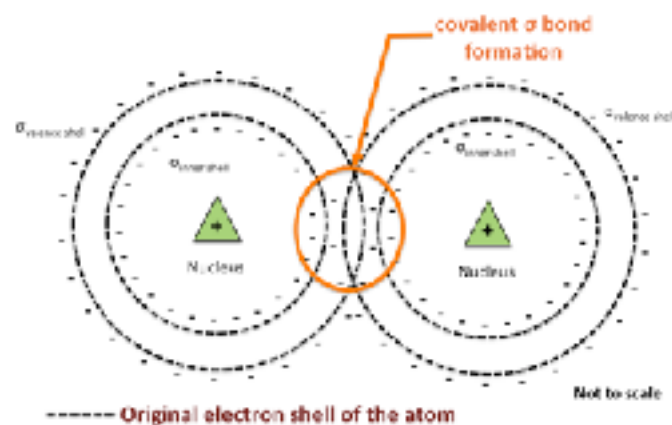
### 10.3.1 Overlapping of the electron shells at bonding

The two opposite charges, nucleus, and electrons, are in electrostatic equilibrium in the atom. In each periods new surface charge electron shell is formed (chapter 6). Disturbing the equilibrium of the non-revolving surface charge electron shell induces ripples on its surface. These ripples propagate as waves in the surface charge electron shell. It has been shown for the Hydrogen atom that the velocity of the traveling wave in the surface charge electron shell is identical with the calculated velocity of the orbiting electron in the Bohr's model (Garai 2017).

The propagating wave in the surface charge electron shell indicates that the electron shell is able to resist tensile strength. For the existence of covalent bonds, this is a fundamental criteria, since otherwise the bond would be non-saturated. When two neutral atoms collide, then the two valence charge electron shells of the neutral atoms start to overlap, and the two valence electron shells trap each other forming a  $\sigma$  bond (Fig. 10.5).

#### *The formation of $\sigma$ bonds*

The overlapping of the electron shells of the atoms has two effects. The nucleus attracts the overlapped surface charge valence electron shell of the captured atom and the inner or core electron shell repels it. The attractions of the nuclei hold the mutually trapped electron shells of the atoms, while the repulsion of the inner shells or core electrons stabilizes the position of the attracted shells (Fig. 10.5). The force holding the trapped part of the electron shell is transferred through the strength of the surface charge shell, which holds the entire atom in a stable position. This kind of bond formation requires that both atoms must have at least two electron shells. The presented simplified description of sigma bond model can be tested by detailed electrostatic analysis.



**Figure 10.5** The schematic of the  $\sigma$  bond. The overlapping, trapped surface charge electron shells of the atoms form a  $\sigma$  bond. The nucleus attracts the trapped surface charge valence shell of the atom and the inner electron shell repels it.

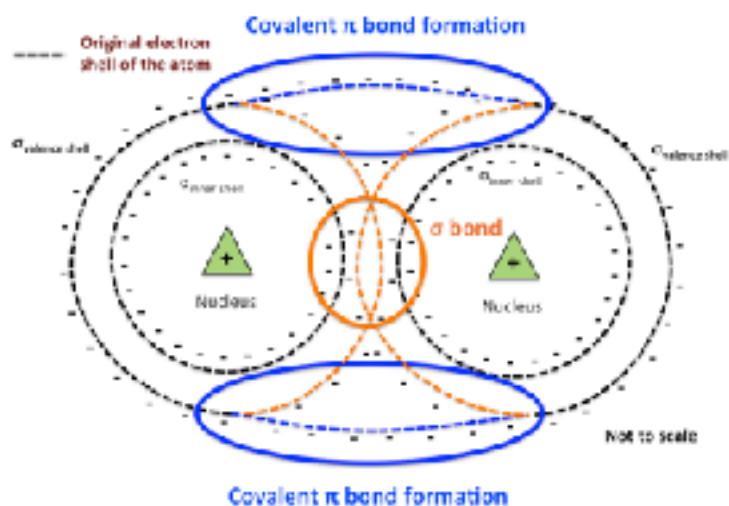
Lewis's empirical postulation, the sharing of electrons of the atoms forming a bond, points in the right direction but his original proposal needs to be refined. The bond is formed when the overlapping non-revolving surface charge electron shells are trapped under the attraction of the nuclei of the other atom.

The overlapping electron shell model of covalent bonds is supported by experiments, which show that the volume of a bonding electron pair is always smaller than the volume of a non-bonding electron pair.

#### *The formation of $\pi$ bonds*

Following the formation of  $\sigma$  bonds, the simultaneous attractions of the two nuclei on the two shared surface charge electron shells can also form additional bonds between two atoms (Fig. 10.6). Based on convention this type of bond formation is called  $\pi$  bonding. The  $\pi$  bond formation should always be preceded with the formation of  $\sigma$  bonds with the exception of the first row of the periodic table, where the atoms have only one electron shell. This prediction is consistent with energy calculation for the formation of  $\pi$  bonds, which requires fulfilling the  $\sigma$  bond energy levels first. If the sharing of electron shells is prevented by the existence of additional  $\sigma$  bonds then  $\pi$  bonding will not be formed. In this case the atoms form hybrid bonds, like the carbon atom in methane form  $sp^3$  hybrid bonds.

Quantum mechanics predicts that the electron density of the  $\pi$  bonds should resemble a locus shape. Experiments detect circular shape, which contradict with quantum mechanical prediction (Berkovitch-Yellin and Leiserowitz 1975). The non-revolving surface charge electron shell model is consistent with the experimentally detected circular formation of  $\pi$  bonds.



**Figure 10.6** The schematic of  $\pi$  bond. Following the formation of  $\sigma$  bonds the additional charges in the valence shell can be shared and under the attraction of the nuclei forming  $\pi$  bonds.

### 10.3.2 Order of bond formation

When the two valence electron shells of the atoms encounter then based on geometrical constrain  $\sigma$  bond must be formed first (Fig.10.6). The  $\pi$  bond/s can only be formed following the formation of the  $\sigma$  bond.

### 10.3.3 Saturation of the bond

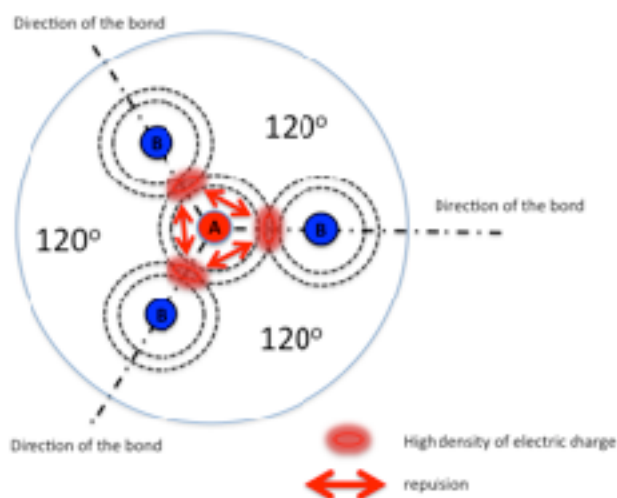
In pure covalent bonds, when the bonded atoms have the same electronegativity, the trapped overlapping electron shells of the two atoms in case of  $\sigma$  bonds have the same charge densities. The same charge densities shield the attraction of the nucleus, which makes the bond neutral outside of the bonding. When a  $\pi$  bond is formed then the joint electron shell of the two atoms with their balanced charges also neutralizes the bond. The presented physical model of the bond formation is consistent with the experimentally verified saturations of the  $\sigma$  and the  $\pi$  bonds.

### 10.3.4 Valence Shell Electron Pair Repulsion (VSEPR)

Atoms forming non-polar purely covalent bonds, in which both atoms have the same electronegativity, are neutral. However, this neutrality does not hold inside the atoms, where the overlapping electron shells induce different charge densities. The repulsions among the various charge density sections are not uniform. Based on electrostatics the regions with the same charge repel each other and moderately destabilize the valence shell. The highest charge density regions are the locations of the bond formation, where the surface charge electrons shells of the atoms are overlapping each other. Thus, within the molecules these regions will be forced to distance out (Fig. 10.7).

Assuming uniform charge density for the lone electron pairs, results in stronger repulsion, compared to the same charge section, where the same charge concentrates in the center of the bond. Thus, the repulsion among the charge sections should be the strongest between two lone electron pairs, medium between bonding and lone pairs, and the lowest between two bonding electron pairs. This outcome of the model is consistent with experiments. The repulsion based on the different charge density of

the regions inside the molecule explains the experimentally verified dimensionality of covalent bonds. This physical explanation of VSEPR is almost identical with the one proposed by Lewis. The difference between the two models is that the repulsion is not the result of electron pairs but rather resulting from the different electron densities of the regions of the molecule.



**Figure 10.7** Schematic 2D figure showing the high charge density regions and their influence on the orientations of the bonds for a planar molecule. The three covalent bonds, in a planar molecule with no lone pair electrons, result in a 120° planar arrangement of the atoms.

### 10.3.5 Delocalization of the electrons

The current point charge electron models of the atoms cannot explain the observed delocalization of the electrons since it would require the fragmentation of the electrons. The valence electrons in the surface charge electron shell model have continuous distribution. For  $\pi$  bonds, where the two valence shells of the atoms jointly forming the bond, partial sharing of the charge of the electron shell is physically possible. Thus, the delocalization of electrons can occur in  $\pi$  bonds, when the bond is formed by the joint surface charge of the valence shells (Fig. 10.6). The experimentally verified delocalization of the electrons is also consistent with the non-revolving surface charge electron shell atom model.

### 10.3.6 Bond electron density

Based on experiments the electron density of the bonds is about 0.1 electrons per bond (ex. Berkovitch-Yellin and Leiserowitz 1975; Dunitz 1983). This electron density increase is emerging from the trapped joint valence electron shells formation of the  $\sigma$  bond/s, and from the jointly shared electron shells of the  $\pi$  bond/s. The theoretically predicted electron density increase of the bonds is consistent with experiments.

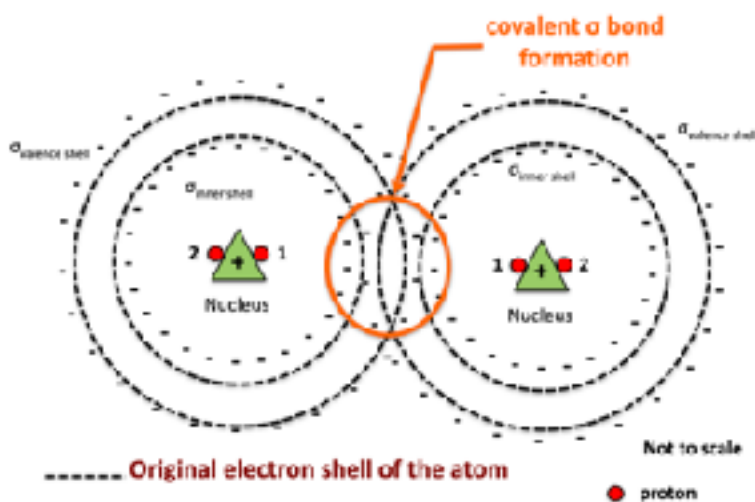
### 10.3.7 Potential models

The attraction of the positive nucleus, on the trapped valence shell of the atom, results in the bond formation. The repulsion of the core electron shells stabilizes the position of the trapped valence shell. The basic features of the two classical potential models are consistent with the physical outcomes deduced from the bond formation of the surface charge electron shell atom model.

### 10.3.8 Bond Dissociation Energy

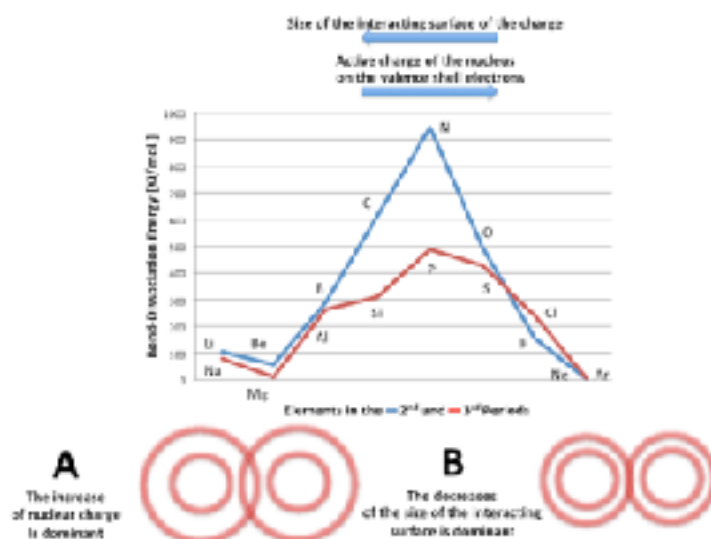
The bond dissociation energy depends on the charge of the nucleus acting on the valence shell and the charge of the valence electron shell, which is the same for neutral atoms. The increase of the non-shielded nucleus charge increases the attraction on the valence shell resulting in stronger bonds. The stronger attraction of the nucleus on the valence shell also reduces the size of the trapped valence electron shells. Thus, the effective size of the interacting valence shells of the atom becomes smaller as the non-shielded nucleus charge increases (Fig. 10.9). If the active interacting size of the two valence electron shells, participating in the bonding, is reduced then the strength of the nucleus attraction becomes smaller. These two contributing factors, stronger attraction by the non-shielded nucleus charge and the reduced active surface area of the bond, have an opposite effect on the bond dissociation energy. The highest bond dissociation energy occurs at the optimum of these two contributing factors.

Besides these two dominant factors, there is a contribution to the bond dissociation energy from the positions of the protons in the nuclear lattice. In each even number nuclei, the added proton of the even number nucleus gets a slightly further away from the bond than the proton in the odd number nuclei (Fig. 10.8). Consequently, the contribution of the even number nuclei to the bond strength is smaller than the protons of the odd number nuclei.



**Figure 10.8** The effect of the position of the protons in the nuclear lattice is shown. Protons of the odd number nuclei (1) are closer to the bond than protons in the even number nuclei (2).

The characteristic trend of the dissociation energies plotted for the elements is consistent with this proposed physical explanations (Fig. 10.9).



**Figure 10.9** The bond dissociation energy of the elements increases with the number of active “non-shielded” proton attraction on the valence shell electrons (A), and decreases with the reduction of the active surface area of the trapped electron shells (B). When process A is the dominant one then the dissociation energy increases, while it starts to decrease when process B becomes dominant. The stronger attraction of the protons for odd atomic number elements has also contribution to the two major factors defining the strength of the bonds.

## 10.4 Conclusions

The presented physical explanations for covalent bonds refine Lewis theory. Lewis described covalent bonds as: Covalent bonds are definite physical reality where “something” binds the atom to atom. The only modification that should be added to this description is that the “something” should be specified as “the attraction of the nucleus on the trapped valence electron shells of the atoms”.

It has been shown that the non-revolving surface charge electron shell atom model is consistent with all of the features of the covalent bonds and offers feasible physical explanations for them. The presented covalent bond model can be tested by classical electrostatic, even though, the calculations are not trivial because the bonds cannot be analyzed using Gaussian surfaces.

## References to Chapter 10

This chapter was presented at 27<sup>th</sup> annual Conference of The International Society for the Philosophy of Chemistry in 2024.

\*Garai, J., The surface charge electron shell atomic model consistent with all the features of covalent bonds, Book of abstracts of the 27<sup>th</sup> annual Conference of The International Society for the Philosophy of Chemistry (ISPC 2024) July 15-17 2024, Varazdin, Croatia

Berkovitch-Yellin, Z., Leiserowitz, L.: Electron density distribution in cumulenes. Low temperature x-ray study of tetraphenylbutatriene. *Journal of the American Chemical Society* **97**(19) 5627-5628 (1975) doi.org/10.1021/ja00852a075

Dunitz, J. D., Schweitzer, B.W., Seiler, P.: X-ray Study of the Deformation Density in Tetrafluoro terephalodinitrile : Weak Bonding Density in the C, F-Bond. *Helvetica Chimica Acta* **66**(1) 123-133 (1983)

Garai, J.: Mathematical Formulas Describing the Sequences of the Periodic Table. *Int. J. Quantum Chem.* **108**, 667-670 (2008)

Garai, J.: The electronic structures of the atoms. *Physics Essays* **30**(4), 455-460 (2017)

- Garai, J.: Nuclear Lattice Model and the Electronic Configuration of the Chemical Elements, Chapter 2 in Mendeleev to Oganesson A Multidisciplinary Perspective on the Periodic Table, Ed. E. Scerri and G. Restrepo, Oxford University Press (2018)
- Garai, J.: Atomic Structure: Validation of the Electron Phase Transformation Theory. *Chem. Sci. Int. J.* **32**(6), 78-98 (2023b)
- Garai, J.: Examining the Electron Phase Transformation Theory in the Context of Atomic Structure. *Chem. Sci. Int. J.* **33**(4) 11-18 (2024a)
- Garai, J.: The phase transformation of the electron forms and atomic capacitor, *Physics Essays* **37**, 3, 200-201 (2024b)
- Heitler, W., London, F.: Wechselwirkung neutraler Atome und homopolare Bindung nach der Quantenmechanik. *Zeitschrift für Physik*, **44**, 455-472. (1927)
- Lennard-Jones, J.E.: Cohesion. *Proc. Phys. Soc.* **43**, 461-482 (1931)
- Lewis, G. N.: The Atom and Molecule. *J. Am. Chem. Soc.*, **38**, 762-785 (1916)
- Morse, P.M.: Diatomic molecules according to the wave mechanics. II. Vibrational levels. *Phys. Rev.* **34**, 57-64 (1929)
- Needham, P.: The source of chemical bonding. *studies in History and Philosophy of Science* **45**, 1-13 (2014)
- Nordholm, S., Bacskay, G.B.: The Basics of Covalent Bonding in Terms of Energy and Dynamics. *Molecules* **25**(11) 2667 (2020) doi.org/10.3390/molecules25112667
- Rumble, J., Bruno, T.J., Doa, M.J.: *CRC Handbook of Chemistry and Physics 104<sup>th</sup> Edition*, CRC Press (2023)
- Scerri, E. R.: On the nature of chemical bonding. Plenary talk at the 26<sup>th</sup> Conference of the International Society for the Philosophy of Chemistry, Lille University, France, virtual, August 15-21 (2022)
- Scerri, E. R.: A commentary on Weisberg's critique of the structural conception of chemical bonding. *Foundations of Chemistry* **25**, 253-264 (2023)
- Seifert, V.A.: The Chemical Bond is a Real Pattern. *Philos. Sci.* **90**, 269-287 (2023)
- Zhao, L., Schwartz, W.H.E., Frenking, G.: The Lewis electron-pair bonding model: the physical background, one century later. *Nature Reviews Chemistry* **3**, 35-47 (2019/a) doi.org/10.1038/s41570-018-0052-4
- Zhao, L., Pan, S., Holzmann, N., Schwerdtfeger, P., and Frenking, G.: Chemical Bonding and Bonding Models of Main-Group Compounds. *Chem. Rev.* **119**(14) 8781-8845 (2019/b) doi.org/10.1021/acs.chemrev.8b00722
- Weisberg, M.: Challenges to the Structural concept of Chemical Bonding. *Philos Sci* **75**, 932-946 (2008)

## 11. Concluding remarks

Based on previous publications of the author, a completely new description for the atomic structure of the chemical elements is presented in the book. The three underlying assumptions of the proposed atom model are:

One, the properties of the chemical elements are identical and invariant, which can only be ensured if the charge distribution of the nucleus for each of the elements are identical. This requires a lattice arrangement of the nucleons.

Two, classical electromagnetism is valid at atomic scale. There is no theoretical base to discredit classical electromagnetism at atomic scale, and experiments are consistent with its validity.

Three, the opposite charges in the atoms are in static equilibrium. Dynamic equilibrium in the time scale of the universe would be chaotic, which would contradict with the known stability of the atoms.

Protons and neutrons have the same size, and they should occupy the space most effectively, which is the closest packing arrangement. The building block of the closest packing arrangement is tetrahedron, containing four nucleons. Helium completes the first period of the periodic table, with the same number of nucleons. Expanding this tetrahedron unit, the number of protons in the added layers of the tetrahedron are the same as the number of elements in the periods. Developing a double tetrahedron nuclear structure reproduces the periodicity of the elements.

The chemical properties of the elements defined by the number of the unshielded protons and the positions of these protons in the lattice. The electronic structure of the elements follows the structural development of the nucleus, governed by the distance between a newly added proton in the nucleus and the valence electron shell. New shell is formed when the attraction of the added proton of an element is smaller than the previous one, which prevents the captured electron to join to the existing electron shell. The geometry of the tetrahedron nucleus is consistent with this assumption. Electronegativity is the outcome of the positions of the protons in the nuclear lattice, which even offers a physical explanations for the irregularities.

The stationary equilibrium of the opposite charges can only be maintained, if at least one of the charges is a distributed one. In order to ensure the stability of the atoms the point charge free (unbounded) electrons at capturing has to be transferred to a surface charge electron shell around the nucleus, and vice versa. This phase transformation of the electrons is energetically feasible, and supported by the different behavior of the free and bounded electrons. The surface charge electron shell model also offers a comprehensive theoretical explanation for the formation of the covalent bonds.

The author hopes that the readers have been convinced a paradigm shift in our understanding of the atomic structure of the chemical elements is necessary.