Graphical 3D Modeling and Analysis of Molecules and Nanostructures with the BSM-SG Atomic Models

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Abstract: Nanostructures exhibit physical properties not predictable by Quantum mechanics, which deals explicitly with energy levels. Trying to work with physical dimensions is a problem not solved from the time of adoption of the Rutherford-Bohr model of hydrogen. Quantum mechanics also does not predict the chemical bond direction, it cannot provide a classical explanation of the spin of leptons and hadrons, why some isotopes are stable and others not, why the neutron has a magnetic moment and the electron has anomalous one, what is the size of the Rydberg state of atoms and so on. Quantum mechanics is also unable to explain the nuclear transmutations at low temperature or so called LENR processes. These and other problems lead to the conclusion that the Quantum mechanics is not a real physical but a mathematical model only. The reexamination of the scattering experiments also leads to this conclusion, since the spherical shape of the nucleus has been a priory used in the data interpretation. The physical models derived in the Basic Structure of Matter Supergravitation Unified Theory (BSM-SG) provide classical explanations of all these problems. The BSM-SG atomic models, provided in the Atlas of of Atomic Nuclear Structures are suitable for 3D graphical modeling and analysis of molecules and nanostructures at sub-nanometric scale. A clickable Periodic table of BSM-SG models is available on-line: www.helical-structures.org/Heliconstruct/table.html

Keywords: nanostructures, sub-nanometer scale, BSM-SG atomic models

1. Introduction

Nanostructures exhibit physical properties which are not predicted by Quantum mechanics (QM). Do QM models of the atoms and elementary particles correspond to physical reality or they are only mathematical? QM atomic models are based on the Rutherford-Bohr planetary model of hydrogen that has unsolved problems from the time of its adoption:

- What is the size of the exited atoms before ionization (Rydberg state)? For quantum number approaching infinity, the size grows to infinity (boundary definition problem)
- Why the orbiting electron does not radiate?
- Is there a classical explanation of the constant electrical charge?
- What does define the spin of elementary particles, while they are assumed spherical?
- How to explain the nuclear spin and spin number if the nucleus is spherical?
- Why the Periodic table has such a shape with separated rows of Lanthanides and Actinides?
- Why some isotopes are stable and others not?
- What physical condition defines the length and angular direction of the chemical bonds in molecules?
- Why the neutron has a magnetic moment and the electron exhibits an anomalous magnetic moment?

Quantum mechanics avoids the discussion on the above-mentioned problems. The rescue argument is that the human logic fails in QM explanation. Such imposed belief is an obstacle for logical understanding of many phenomena in microscale, including some observed effects in nuclear transmutations and nanotechnology.

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2. Investigating the scattering experiments

The QM models of atoms are based on the Bohr model of the hydrogen adopted in the beginning of 19th century. Based on a planetary-like model, it assumes a very small nuclei, however the problems known from the time of its adoption, are not resolved. As a result, the Quantum Mechanics postulated using only energy levels. Any attempt to work with dimensions of the atoms, even for the hydrogen leads to huge inconsistencies. This led to the imposed belief that the human logic cannot work at the microcosmos level where quantum mechanical interactions take place. The interpretation of scattering experiments from the time of Rutherford is also based on the assumption of the planetary models of the atoms. In such way they wrongly lead to a very small atomic nucleus. They don't have a transversal resolution, but only an angular one. If simply assume that the shape of the hadrons that build the nucleus, for example, is not a sphere but a twisted or folded torus, thinner but larger the scattering data will be the same. But then the near Coulomb field will be spread at much larger volume and the problem of overcoming the Coulomb barrier becomes quite different. Additionally, closer to the atomic nuclei there are strong nuclear forces that make a space microcurvature. This makes some kind of nonlinear space that is dismissed in QM models, but this will also cause a wrong interpretation of the data from scattering experiments. Detailed discussion about the scattering experiment misinterpretation is provided in [1].

3. A new approach:

The Basic Structures of Matter – Supergravitation Unified Theory (BSM-SG) is based on alternative concept of the physical vacuum [2,3,4]. The theoretical analysis of the experiments and observations reveals the existence of superfine underline structure of the physical vacuum, called a Cosmic Lattice. At microscale range the Supergravitational (SG) forces play a role of nuclear forces and they are able also to modify the Coulomb field. At macroscale range the SG forces are propagated through the Cosmic lattice and manifest themselves as a Newtonian gravity. The revealed material shapes of elementary particles and atomic nuclei are not spherical. Their features permit classical explanation of all above-mentioned problems.

All elementary particles according to the BSM-SG possess helical substructures with properties to create a charge by specific modulation of the space fabrics (physical vacuum)

Proton and neutron possess one and a same superdens substructure but with different overall shapes. The proton is a twisted torus, while the neutron is double folded. The charge of the neutron is locked in the near field by the SG (nuclear) forces and not detectable, but when in motion it creates a magnetic field. Dimensions are derived by analysis of the particle physics data and experiments, the molecular spectra and the revealed structure of the electron. They are verified by experimentally known data of chemical bonds. Fig. 1. shows the shape of the neutron and proton with their near electrical field and how they form the deuterium.

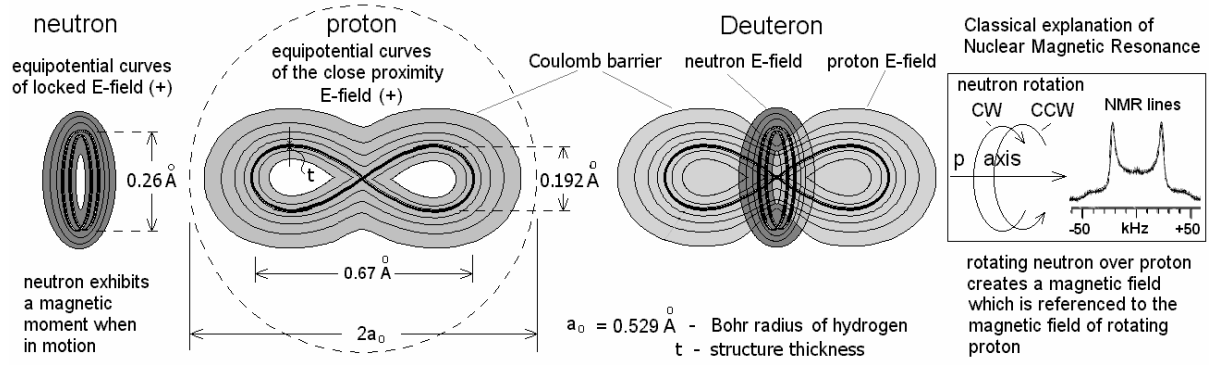


Fig. 1. Shape of the neutron, proton with their near electrical fields and how they form the deuterium. It also show the classical explanation of the nuclear magnetic resonance of deuterium

While the electrical field of the proton is detectable in the far field, in the neutron this field is locked in the near field by the SG forces, due to its overall shape. It provides a magnetic field only when the

neutron is in translational or rotational motion. This feature helps to make a classical explanation of the nuclear magnetic resonance of deuterium. The magnetic field of rotating neutron interacts with the much stronger magnetic moment of the electron, so this gives the strength of the NMR, while the heavier neutron serves as a flywheel. This feature is further valid for all atoms and provides the stability of the nuclear spin. The nuclear spin and NMR are discussed in [11, §1.3.7]. The BSM-SG models permits to find some connection between the nuclear spin number and the isotope stability. It appears that isotopes with better rotational arrangements of nuclear hadrons in respect to the polar axis are more stable.

Fig. 2 shows the invisible by the electron microscopes material structure of the electron as a small 3-body oscillating system. In external electrical field it exhibits a screw-like motion with preferred quantum velocities (13.6 eV, 3,4 eV, 1.51 eV…) due to phase matching with the oscillating features of the nodes structures of the space fabrics, known in BSM-SG theory as a Cosmic Lattice [5].

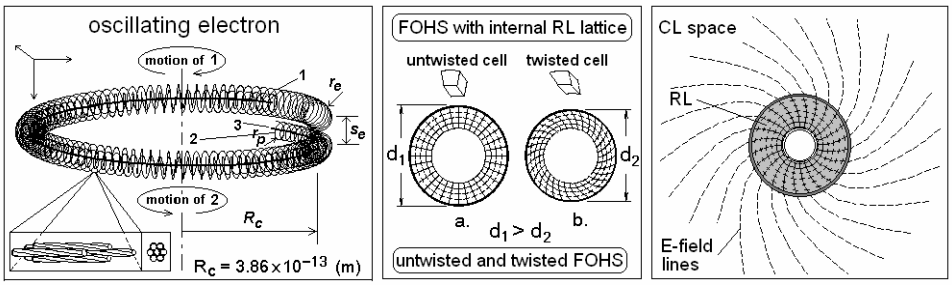


Fig. 2. Internal material structure of the electron, where R_C is the Compton radius.

Fig. 3. illustrates the formation of the first simple atomic nuclei as 3D fractal structures, held by strong nuclear forces, which are called Supergravitational forces in the BSM-SG theory (see Chapter 8 of BSM-SG).

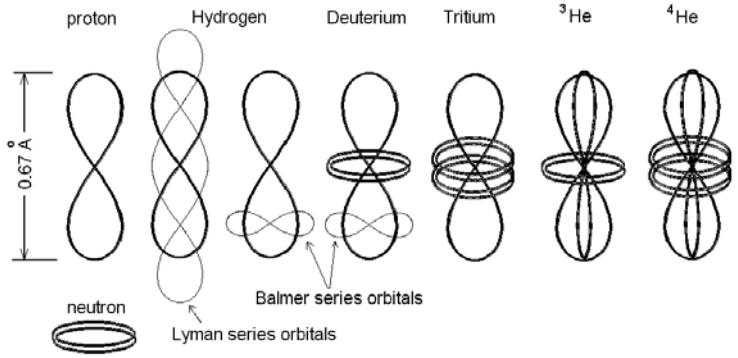


Fig. 3. Stable elementary particles and simple atomic nuclei

Fig. 4. Illustrates the arrangement of the protons and neutrons in the atomic nuclei governed by the SG forces and near field Coulomb forces. The symbolic sign used the proton is like the figure 8, while for the neutron is a crossing line.

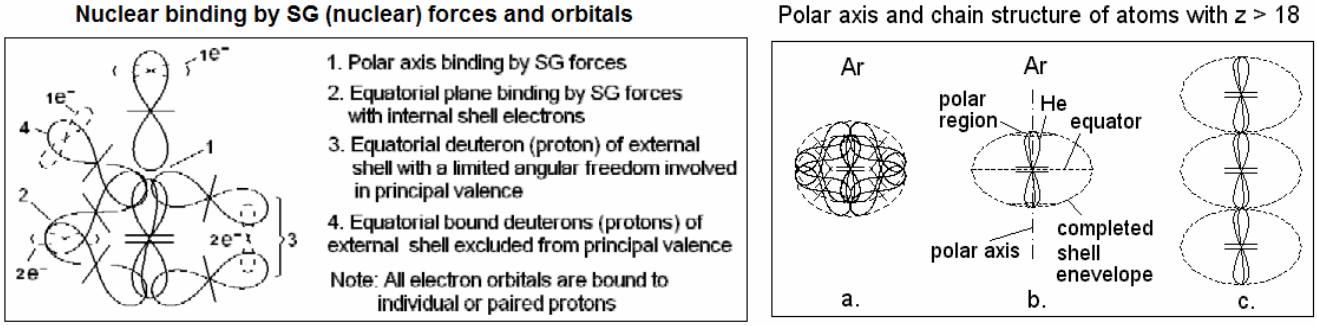


Fig. 4. Nuclear binding forces and chain-like arrangement of hadrons in atomic nuclei. A polar axis is clearly identifiable. Nuclear bonds: 1 – polar SG bond, 2 – equatorial SG bond, 3 – electronic bond. In the chain structure the densest He nuclei are in the middle.

The configuration principle of the atomic nuclei illustrated in Fig. 4 permits understanding the rule of build-up process of the stable elements, which form the pattern of the Periodic Table. It allows understanding the chemical valences, the chemical bond directions and isotope stability. Starting from the first elements from the row, when the z-number increases the principal chemical valence also increases until the deuterons (protons) from the two poles are at different planes passing through the polar axis. In further z increase the deuterons (protons) are met and bound at equatorial region by electronic bond, so they are excluded from the principal valence. At noble gases all deuterons are bound at equatorial region by SG forces and strongly excluded from any chemical valence. Fig. 5. Illustrates the atomic nuclei in two rows of the Periodic table, while Fig. 6 shows the atomic nuclei of some selected elements in two 2D projections.

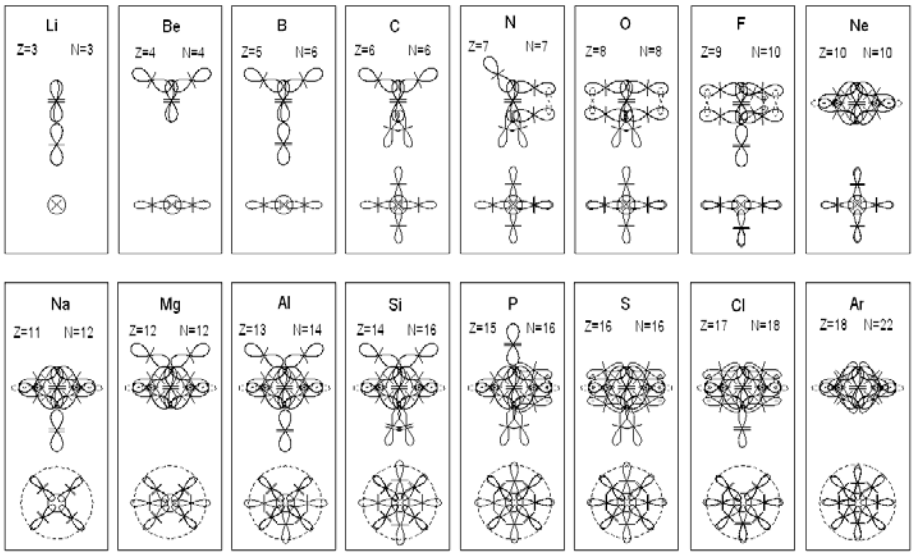


Fig. 5. The atomic nuclei in two rows of the Periodic table.

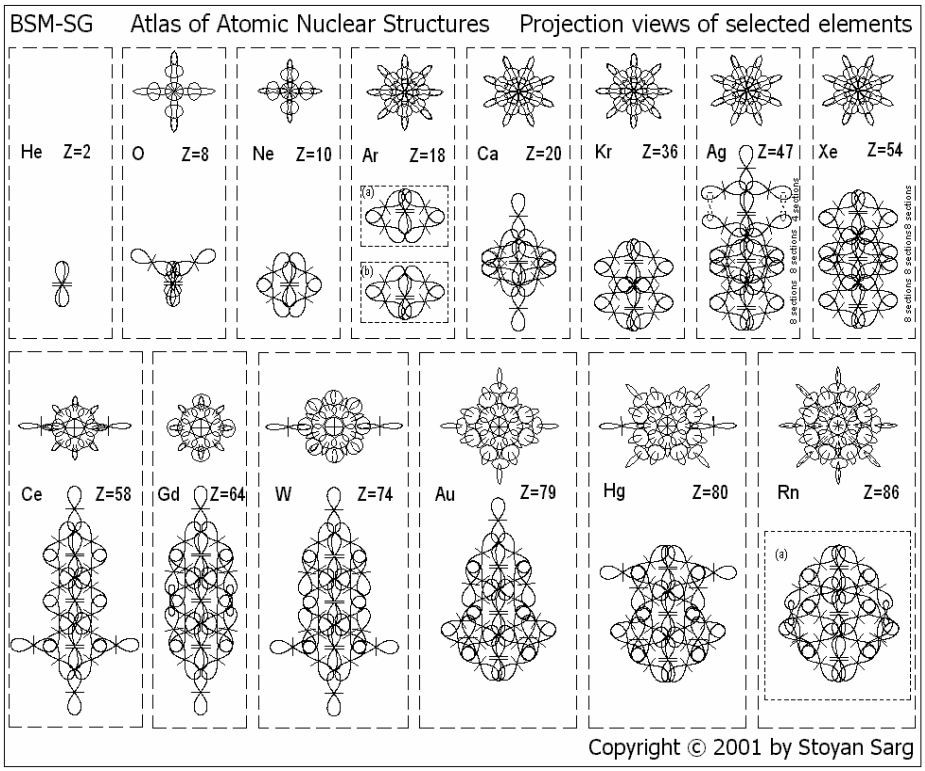


Fig. 6. Atomic nuclei of some selected elements

4. Examples of graphical 3D modeling of molecules in sub-nanometer scale with the BSM-SG atomic models

Fig. 7 illustrates the atomic arrangement in some simple molecules. The chemical bond directions are defined by the nuclear configurations of the valence protons that have restricted angular freedom due to near range Coulomb fields of the protons. For O_2 molecule two different states are shown. They have distinguished vibrational-rotational spectra (see analysis in Chapter 8 of BSM-SG, §9.16). The BSM-SG models leads to the conclusion the Brown gas (HHO) is a specific state of the water molecule, where the two electrons in a common orbit possess a higher quantum energy level. This excludes the mutual H-bond interactions making the HHO molecule a gas at normal temperature. If ignited, the volume of Brown gas implodes because the HHO state converts extremely fast to a normal water molecule. The IR spectrum of HHO is different from the spectrum of H_2O, O_2 and H_2 [6]. Fig. 8. shows a cluster of three water molecules.

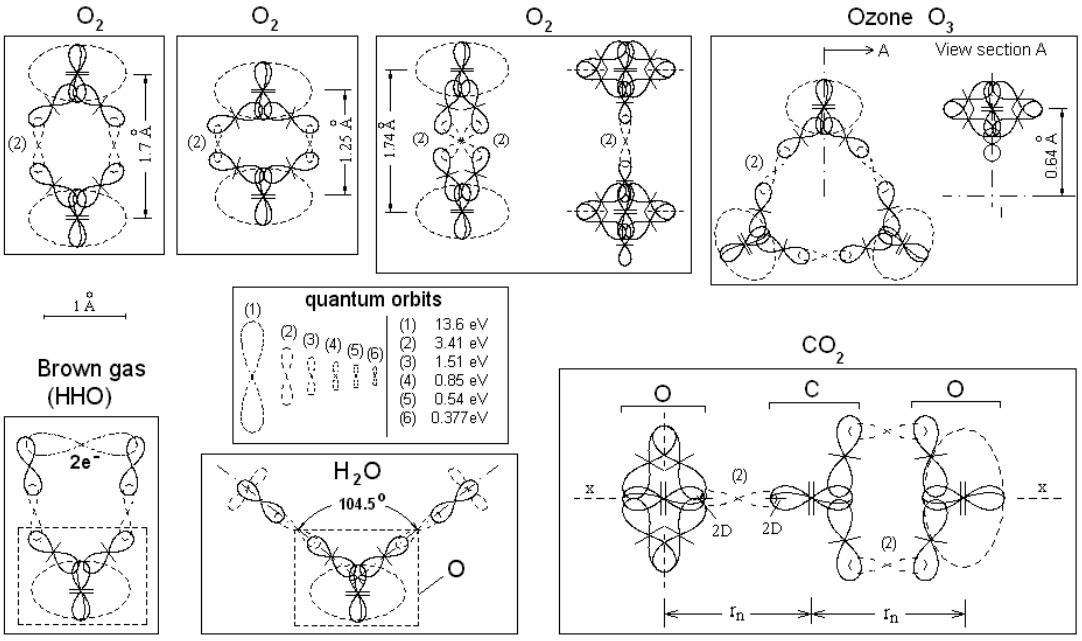


Fig. 7. Atomic arrangement in some simple molecules.

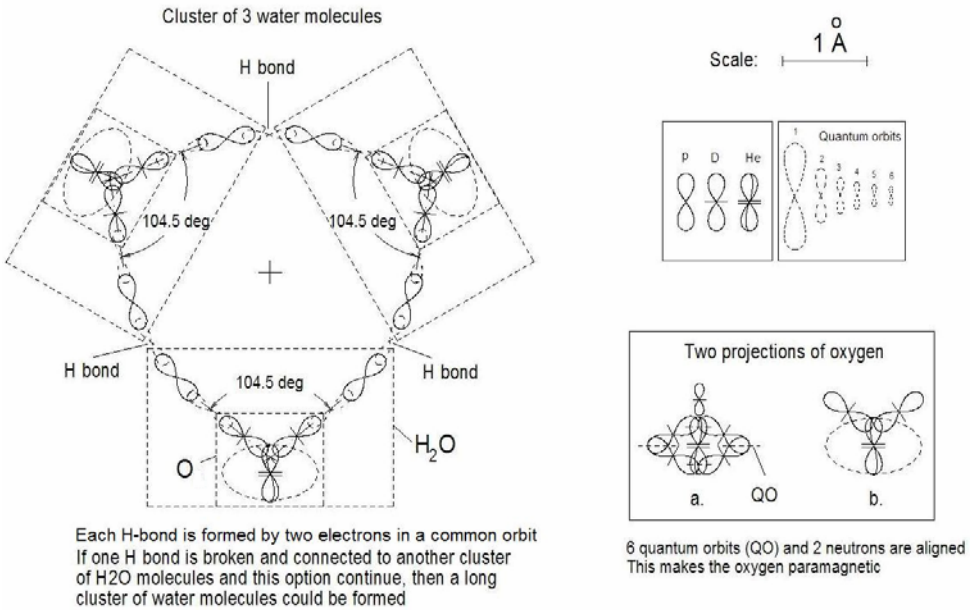


Fig. 8. A cluster of three water molecules, as envisioned by BSM-SG theory. The existence of this cluster is proofed by FIR spectroscopy [7]

One may see from Fig. 8 that all hydrogen bonds of the structure called a water trimer are interconnected and they lie in one plane. Such flat arrangement is favored at the surface of the liquid water and it might play a role in the surface tension.

It is known that the energy eigenvalues of hydrogen (one electron) atom are strongly determined by the principle quantum number, ***n***, and less by the angular momentum, ***l***. For many-electron atoms, however, some energy levels depend stronger on ***l***, than on, ***n***. This means that the magnetic interactions play a strong role. Fig. 9. illustrates the magnetic field interactions from the electron orbitals of the Beryllium neutral atom (two valence electrons) and the beryllium ion (one electron in the external shell).

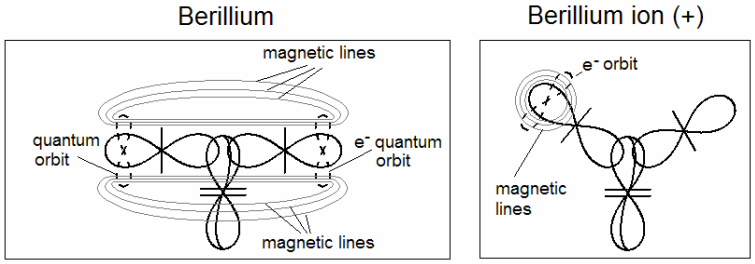


Fig. 9. Magnetic field of the Beryllium neutral atom and beryllium ion.

Fig. 10 shows one interesting feature of the ozone molecule consisting of three oxygen atoms connected in a ring. Magnetic fields of the quantum electron orbits are confined.

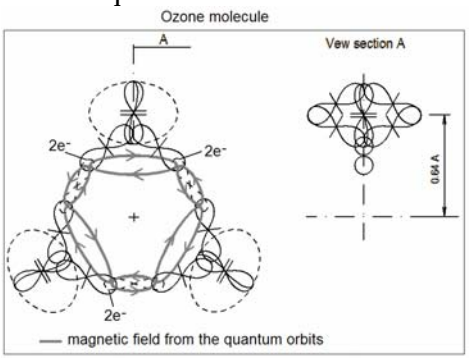


Fig. 10. Ozone molecule. The magnetic fields of the quantum electron orbits are confined

Investigating the level shifts in the Grotrian diagrams (see §8.11, §8.12, Chapter 2 of BSM-SG), a conclusion is derived that the elements with more than one electron possess a property of energy storage due to the magnetic coupling between the electronic orbitals. From the similarity of bond connections in molecules a conclusion is made that in molecules formed by ring atomic structures some exited quantum levels will rotate until some external disturbance occurs [8]. Consequently, a molecular structure containing one ore more atomic rings of atoms with more than one principal valence might possess energy well. The molecular structure of aspirin contains such one atomic ring, as illustrated in Fig. 11.

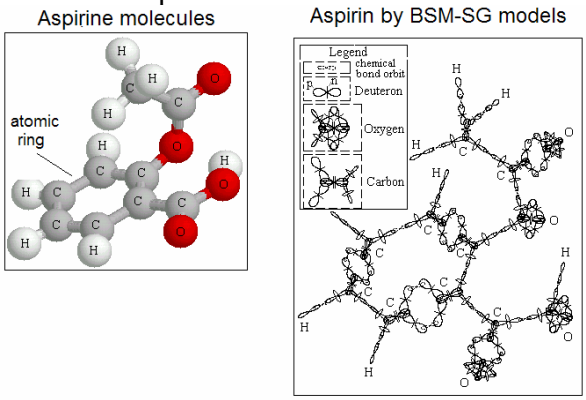


Fig. 11. Atomic ring of six carbon atoms in the molecule of aspirin

Since many proteins and particular the DNA molecule contain an enormous number of atomic rings, we may conclude that they possess an energy saving feature. Fig. 12. shows a portion of DNA strand with an abundant number of atomic rings. At particular moment, which might be triggered by some electrical pulse propagated through the DNA strand, the energy of the DNA atomic rings could be released as an EM radiation carrying the DNA code. A synchronized release of such radiation from the DNA in the neighboring cells will appear as an EM avalanche process possessing a strong penetration property. The avalanche process could be synchronized by the repeating codons in the DNA, known as a C-value paradox. The BSM-SG atomic models allow illustrating also the weak H-bond connections between the two strands of the DNA molecule.

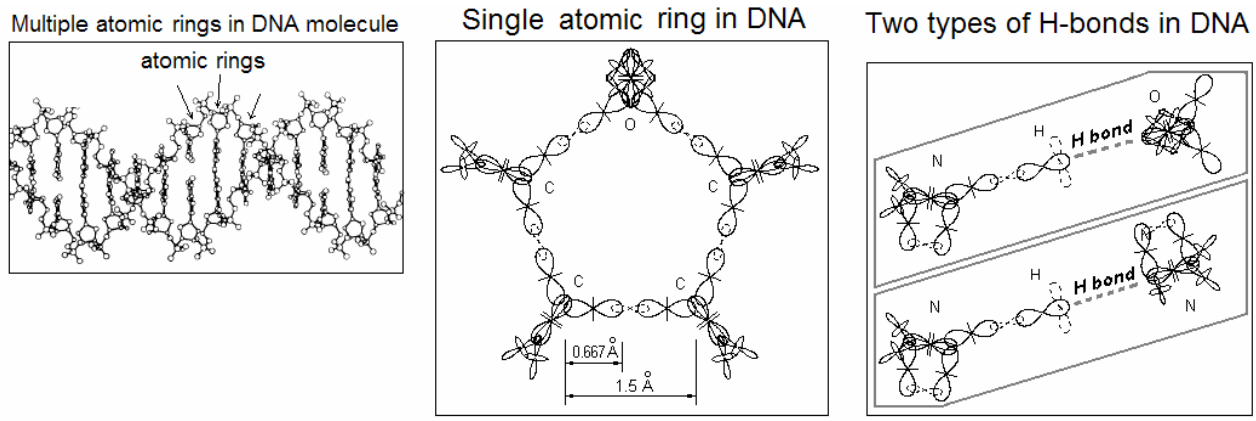
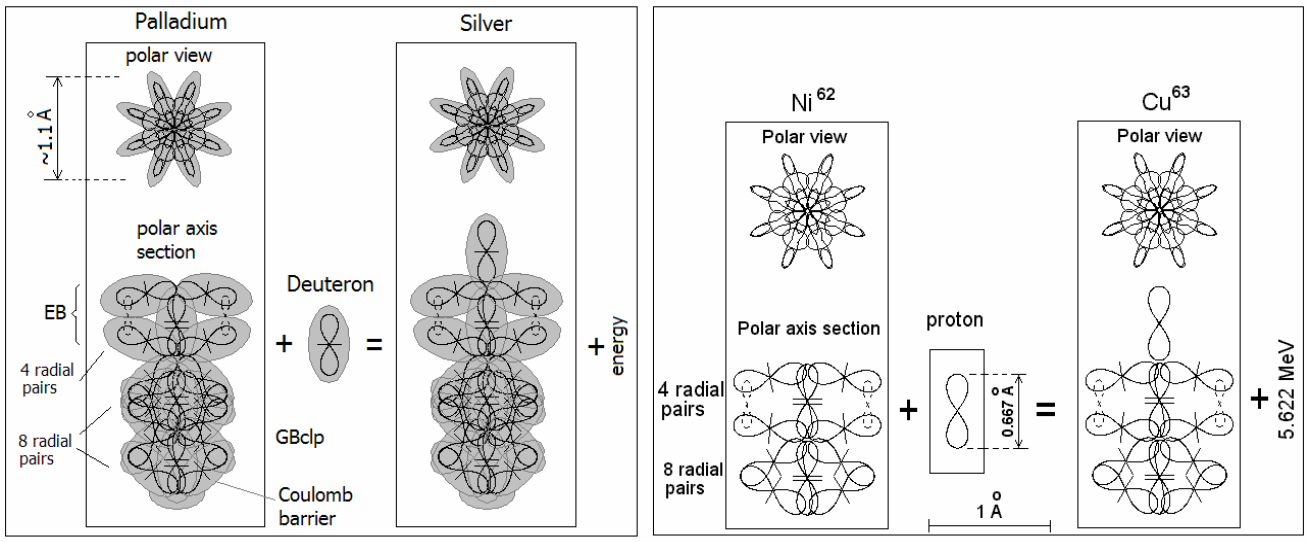


Fig. 12. Atomic rings in DNA molecules and the H-bonds. The weak H-bonds are result of the SG forces at close proximity. They are known also as Wan Der Walls forces.

5. Graphical modeling of nuclear transmutations in LENR

The BS-SG models permits understanding the experimentally observed nuclear transmutations and also some nuclear reactions known as LENR or cold fusion [1,10,11]. This is illustrated in Fig. 13 for two experimentally observed nuclear reactions: Pd + D -> Ag [12] and Mi + H -> Cu [13]. Fig. 14. illustrates nuclear reactions reported by Yasuhiro Iwamura (2012) [14].



a. **b.**

Fig. 13. a. - a nuclear reaction Pd + D -> Ag [12] (the grey pattern shows the near Coulomb field), b. – a nuclear reaction Ni + H -> Cu [13].

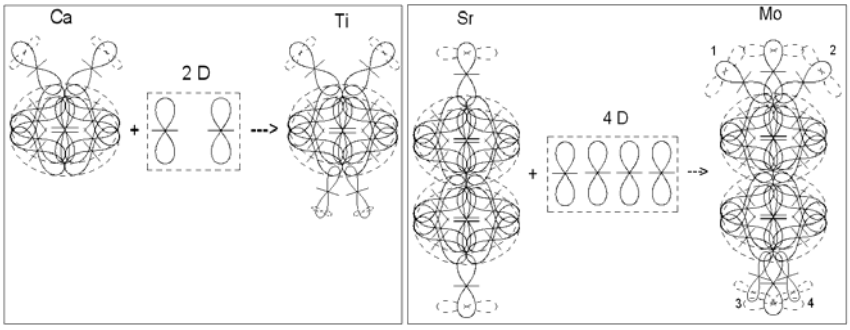


Fig. 14. Nuclear transmutations reported by Yasuhiro Iwamura [14], as presented by BSM-SG models

6. BSM-SG atomic models and nanotechnology

BSM-SG atomic models not only are helpful in understand the atomic arrangement in nanostructures. They could help envisioning some of their properties and even to predict some new nanostructures. Fig. 15 illustrates one example of analysis of the electron microscope image of a graphene sheet.

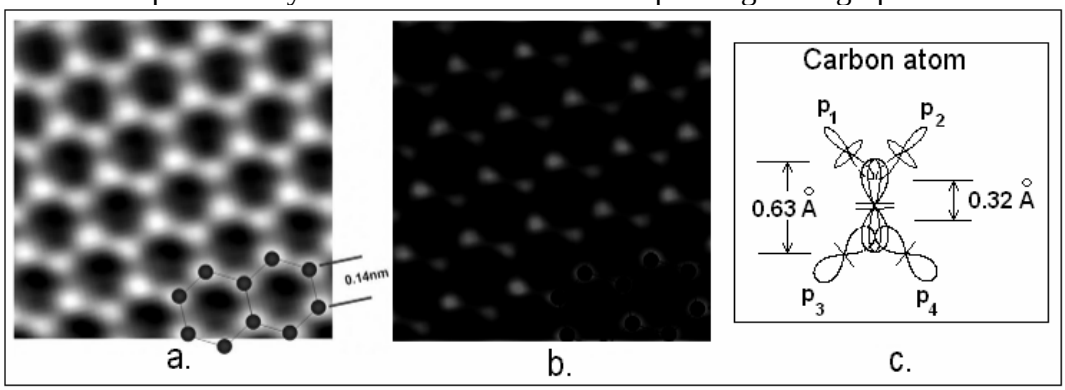


Fig. 15. a – image by TEAM microscope [14], b – processed image by brightness adjustment, c – carbon atom

In the illustrated structure of carbon atom, the plane of P_1 & P_2 is perpendicular to the plane of P_3 &P_4. This provides a slight displacement of the locations of the electronic orbits that in fact connects the free sides of P of neighboring atoms and these local fields are detectable by the electron microscope. As a result, every neighboring white spot in the brightness processed image appears slightly dimmed. Fig. 16 shows the arrangement of the carbon atoms in the graphene sheet using the BSM-SG models.

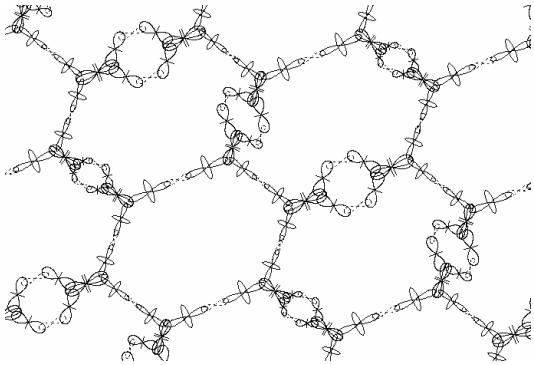


Fig. 16. Carbon atoms in grapheme sheet using the BSM-SG atomic models

Fig. 17. shows electron microscope image of silver nanoparticles with a shape of a tetrahedral observed by R. Jin et al. [15]. The arrangement of silver atoms in one side of the tetrahedral using the BSM-SG atomic models is shown in Fig. 18. Four such triangular sheets of silver nanostructures might form tetrahedrals, as those shown in Fig. 17.

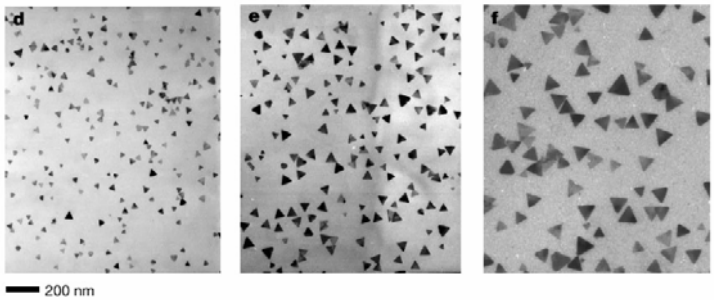


Fig. 17. Electron microscope image of silver nanoparticles. Courtesy of R. Jin et al. Nature 2003 [15]

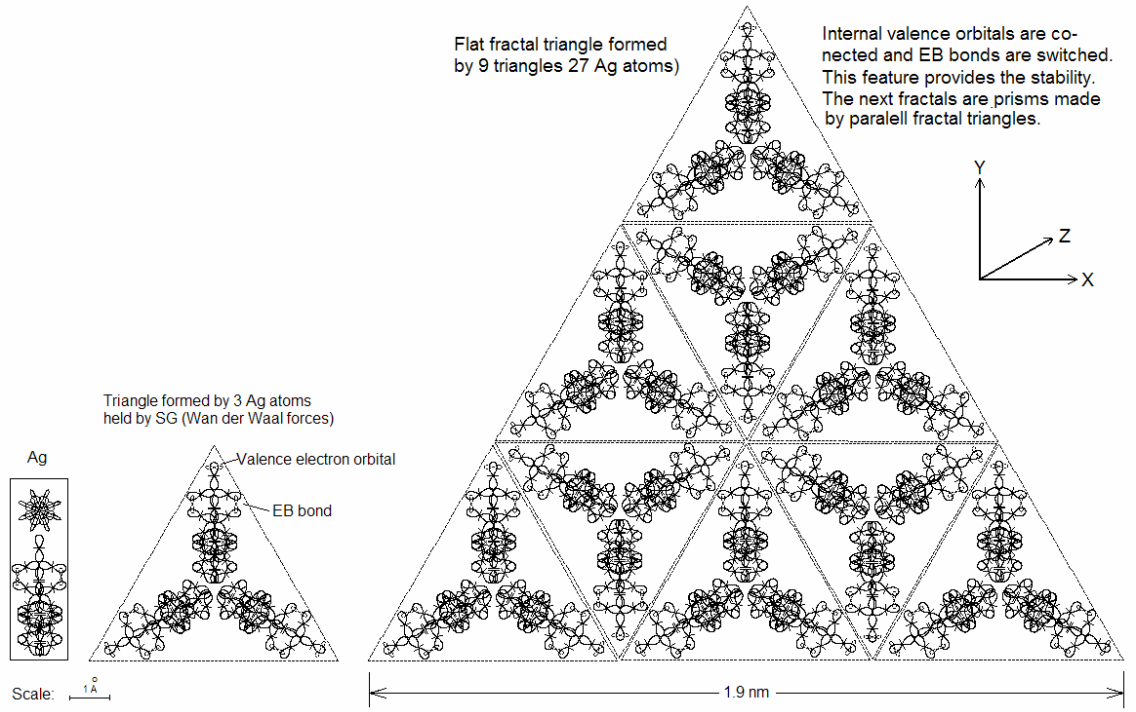


Fig. 18. One side of silver nanostructures, shown as a sheet, illustrated with the BSM-SG atomic models. The left sheet is formed of 3 silver atoms, while the right sheet is formed of 27 silver atoms. The fractal build-up allows obtaining triangular sheets with different sizes in the nanoscale range.

When using the BSM-SG models, as shown in Fig. 18, it is apparent that the silver nanoparticles grow as 3D fractal structures. Single sheets might also exist in so called colloidal silver, which has antibacterial properties due to its average positive charge of two. Using the BSM-SG models it is evident that the valence electrons at the apex could be easier lost and the obtained positive charge will be an average value of two. This is the value observed in the water solution called colloidal silver. The sheet fractal structure may consist of 3, 12, 27 and so on silver atoms, but the average positive charge of 2 will be always preserved.

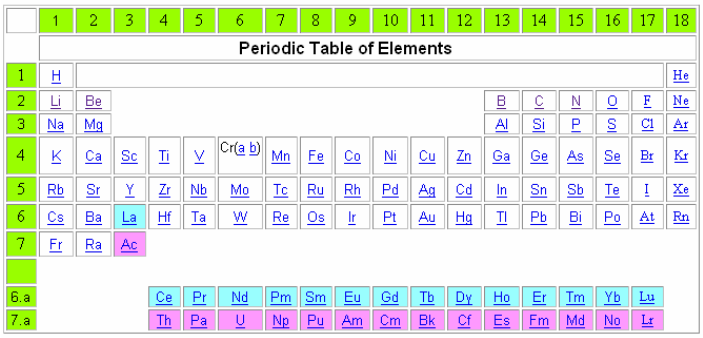


Fig. 19. Clickable periodic Table

The BSM-SG atomic models for elements with $1 < z < 103$, using the are presented in the Atlas of Atomic Nuclear Structures, one of the major contributions of the BSM-SG theory. It is published also as a separate monograph [16,17,18]. Fig. 19 shows a clickable Periodic table, which is available on-line:
www.helical-structures.org/Heliconstruct/table.html

Fig. 20 shows a poster type of the Periodic table of elements using the BSM-SG atomic models.

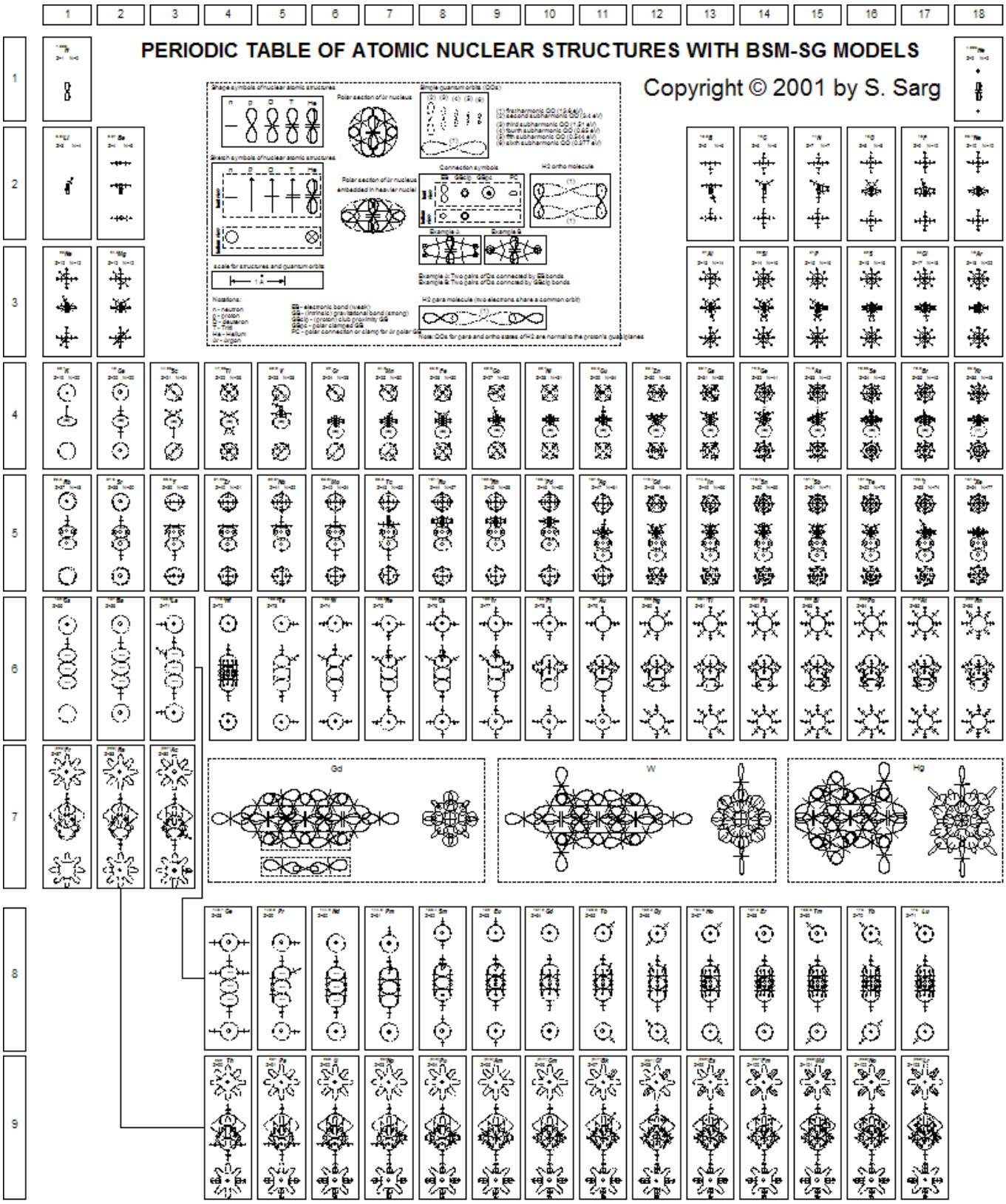


Fig. 20. Periodic table of nuclear atomic structures with BSM-SG atomic models, a poster included in the Atlas of Atomic Nuclear Structures [16,17,18]. For simplicity, the protons and neutrons are shown with symbolic graphical elements: proton - with an arrow and neutron with a line crossing the arrow.

7. Summary and Conclusions

The BSM_SG atomic models permit graphical 3D modeling and analysis of molecules and nanostructures in sub-nanometer scale. They have a potential to be used in the fields of structural chemistry, the nuclear magnetic resonance, identifying the stable isotopes, analysis of LENR and modeling in nanotechnology.

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