Ring models of atoms, molecules and nanomaterials

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Abstract

The classical approach in particle physics is based on the fact that the electron has some parameters like charge, mass, etc. but does not have a structure. In our calculations, the electron is assumed as structured particle having magnetic properties. VFRT (Vortex Fractal Ring Theory) uses the electron, proton, and neutron as a particle with a toroidal (ring) shape, which is formed by fractal substructures connected to each other by vortex electromagnetic fields. The atomic nucleus can be built from the ring protons and neutrons. Combining knowledge of physical chemistry, evolutionary optimization, 3D graphic, programming in Python, and mathematics makes it possible to create programs for designing new nanostructure models. The first testing proposal for the nanostructure prediction program is limited to carbon structures. The aim was to verify whether the proposed program is capable of generating known carbon nanostructures, such as graphene. The following versions of the program will no longer have this limitation.

Keywords: Ring models of nanomaterials, topological ring models of atoms and molecules, ring model of carbon, ring model of graphene.

Introduction

The prediction of new nanostructures requires knowledge of physical chemistry and the ability to select a suitable method of evolutionary optimization. The first such predictor was designed by Organov (USPEX) [**1**], which combines the knowledge of quantum physics and evolutionary optimization. Since quantum physics does not contain a structural description of atoms, this predictor is capable of designing structures with hundreds of atoms on supercomputers. The combination of the structural description of atomic nuclei [**6, 10**, **11**], and grammatical evolution [**7**-**9**] does not have this limitation. The number of atoms of the predicted nanostructure depends only on the performance of the computer and the possible calculation time. The classical approach in particle physics is based on the fact that the electron has some parameters like charge, mass, etc. but does not have a structure. The electron is calculated as point particle having magnetic properties. First and second ionization energies and electron shells are described in [**2**, **3**] and basics of fractal physics are described in [**5**]. Atom radii bond lengths are described in [**4**]. VFRT [**9**-**11**] uses the electron as the fractal particle with a toroidal (ring) shape, which is formed by ring fractal substructures connected to each other by vortex electromagnetic fields. The atomic nucleus can be built from the ring protons and neutrons [**10**].

New VFRT (vortex-fractal-ring-theory) works with the annular structure of the electron, proton, and neutron, and can describe the inner structure of atomic nuclei. The atomic nucleus can be built from the ring protons and neutrons using the following rules [**10**]:

1. The proton cannot be directly connected with the proton, except for two parallel protons with the same axis that are connected together by nuclear forces.
2. Next proton with a different axis can be connected via the coupling neutron to another proton.

Basic substructures of atoms (globules) created from protons and neutrons are in **Fig. 1** (red rings are protons and yellow rings are neutrons) [**10**]. On one axis, there may be a maximum of two protons and two neutrons (and two electrons with opposite spins). It seems that the combination of these two basic rules can create all models of atoms [**10**].

Fig. 1. Globule substructures of atoms created from protons and neutrons (red rings are protons and yellow rings are neutrons) [**10**].

Topological structure of carbon and oxygen nucleus

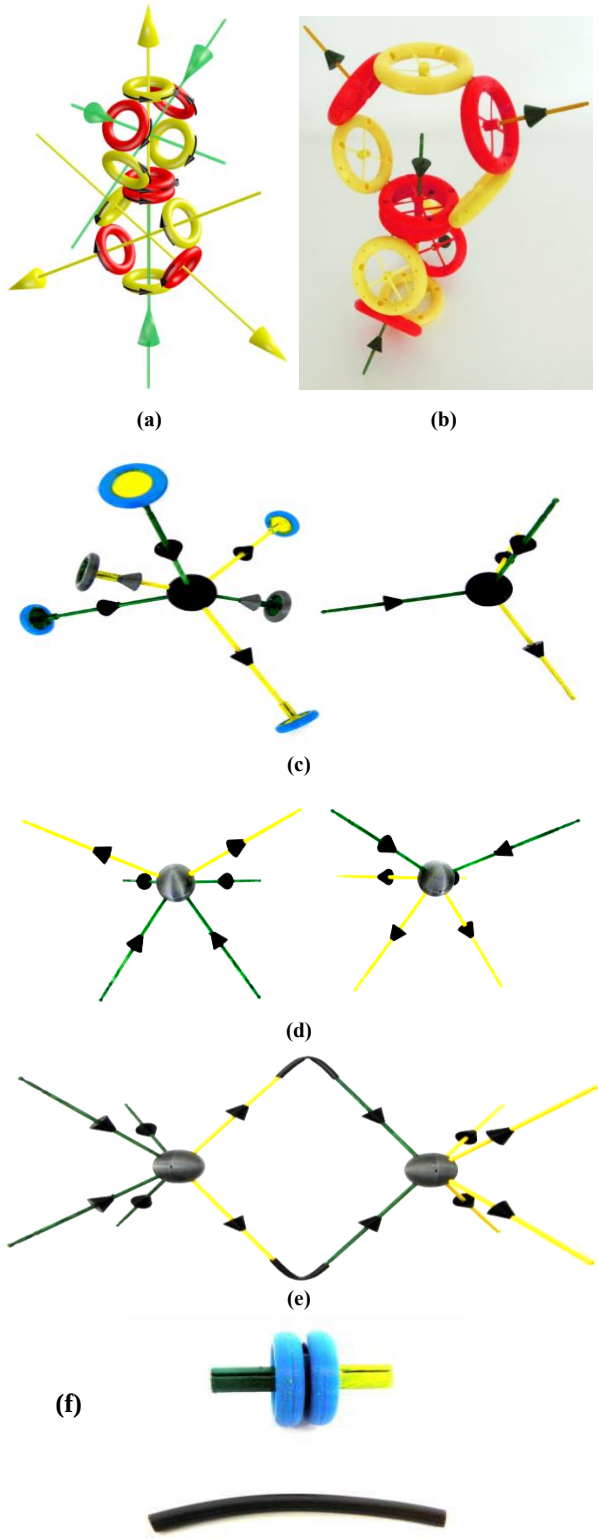

Fig. 2 Topological models: (a) Ring topological structure of carbon nucleus (3D computer model), which consists from two globules with 3 protons (see **Fig. 1**), (b) kit model (educational), (c) Simplification of carbon atom and as a spherical nucleus model which is suitable for grammatical evolution (the arrows determine the directions of the magnetic moments of protons: the outgoing magnetic moments are yellow, the magnetic moments entering are green), (d) Two types of the oxygen nucleus which differ in the opposite directions of magnetic moments, (e) Oxygen molecule (brown connection is covalent bond with two electrons - see (f), (f) Covalent bond with two ring electrons (blue).

Topological ring structures of other atom nuclei are in [**10**], [**11**], [**12**]. Carbon dioxide and methane topological structure are in **Fig. 3**. Red sphere is the nucleus of hydrogen (the proton). Topological models describe structures well but are not in right scale.

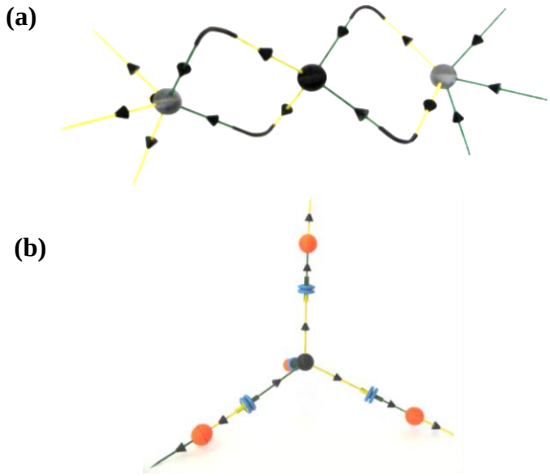

Fig. 3. Topological models (kit): (a) Carbon dioxide, (b) Methane.

Graphene structure and its creation are in **Fig. 4**.

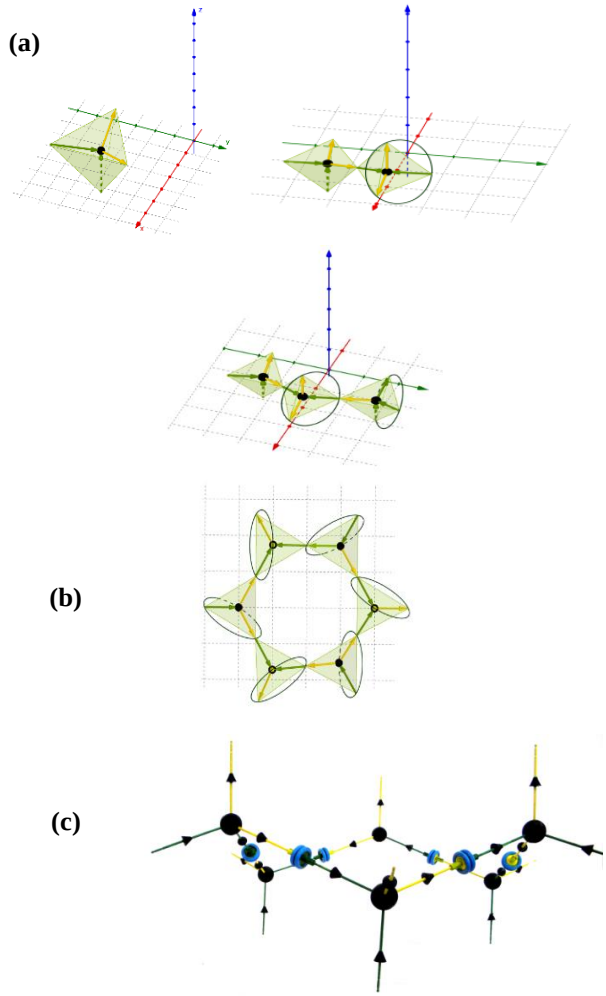

Fig. 4. Graphene: (a) Creation of graphene, (b) 3D computer hexagonal model of graphene, (c) Educational model (kit).

Two hexagonal carbon structures that allow the creation of a graphene structure are in **Fig. 5**. Combining structures H1 and H2 results in a graphene structure - see **Fig. 5c**) [**11**], [**12**]. The number of possible structures is important for defining modulo operation for grammatical evolution rules.

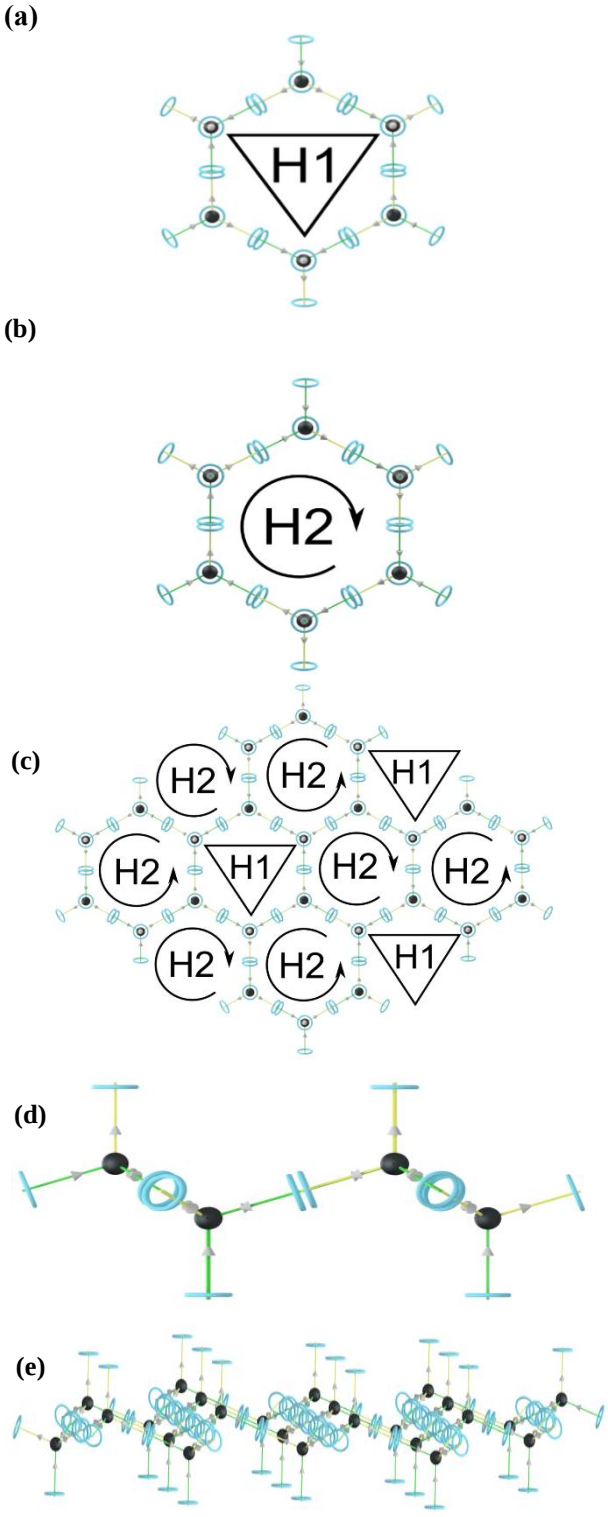

Fig. 5. (a) Hexagonal-topological carbon structures H1 of graphene, (b) Hexagonal-topological carbon structures H2 of graphene, (c) Topological structure of grapheme with H1 and H2, (d) 3D topological model of graphene (side view), (e) Side view of several hexagonal structures.

Grammatical evolution

Basic ideas of grammatical evolution are described in [**7-9**]. In future we will use Grammatical Evolution (GE) with backward processing [**9**]. Translation and crossover are in **Fig. 6**.

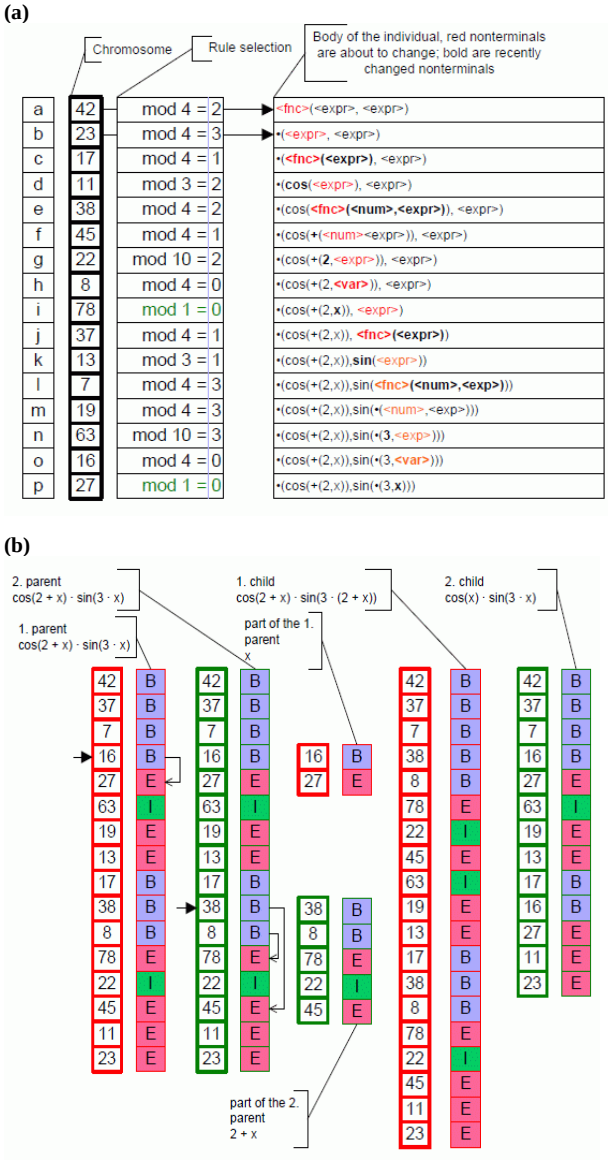

Fig. 6. (a) Translation with back processing, (b) Crossover.

Coding of the chromosome in grammatical evolution

PonyGE2 is an implementation of GE in Python [**8**]. PonyGE2 has the modular structure. Both linear genome representation and derivation tree representation are implemented simultaneously. BNF is notation for expressing a grammar in the form of production rules. Each production rule is composed of left-hand side (a single non-terminal, followed by symbol :: =, followed by a list of production choices separated by the symbol |. Production choices can be composed of any combination of terminals or non-terminals. Non terminals are enclosed by angle brackets <>. For example we consider following production rule:

<*m*> ::= <*i*> | <*o*>. The number of carbon nuclei is gradually increased from 0 to N. The length of the chromosome is gradually extended. Each new bond has the bond energy described in [**2**, **3**] and the bond length described in [**4**]**.** Adding additional carbon atoms gradually increases overall binding energy of the resulting structure, which defines the fitness of phenotype (result of translation genotype from chromosome to phenotype). The best individual in the population has the greatest total coupling energy. Only magnetic moments of the same direction can be connected (see **Fig. 4** and **Fig. 5**). Production rules for design of carbon nanostructures:

N=0,

<*I*> ::= <*a*>,

<*a*> ::= <*k*> <*n*><*m*> <*a*>,

<*n*> ::= *Carbon*,

<*m*> ::= <*i*> | <*o*>,

<*i*> ::= *A* | *B*, <*o*> ::= *C* | *D*,

<*k*> ::= *N*+1,

where, *a* is an atom, *k* is number of the atom, *n* is type of the nucleus (atom), *Carbon* is the nucleus of the carbon, *m* is direction of the magnetic moment, *o* is output direction of the magnetic moment, *i* is input direction of the magnetic moment, *A*, *B* are input magnetic moments of the carbon nucleus, *C*, *D* are output magnetic moments of carbon, *N* is number of atoms during of translation.

Table 1: Coding of derivation tree representation (only carbon nuclei).

Number of nucleus: No:**1**	Type of atom (only carbon, modulo 1)	Used of input/output mg. moment No:	Connected with nucleus No:	Used mg. moment input/output No: in connected nucleus	….

….	Number of nucleus: No:**N**	Type of atom (only carbon, modulo 1)	Used of input/output mg. moment No:	Connected with nucleus No.	Used mg. moment input/output No: in connected nucleus

Calculation of the atomic nucleus position

Vertices of the carbon structure (a regular tetrahedron):

$$V_1[0,0,0], V_2\left[\frac{2\sqrt{6}}{3}c, 0, 0\right],$$

$$V_3\left[\frac{\sqrt{6}}{3}c, \sqrt{2}c, 0\right] \text{ and } V_0\left[\frac{\sqrt{6}}{3}c, \frac{\sqrt{2}}{3}c, \frac{4}{3}c\right],$$

where c is the radius of a sphere circumscribed this tetrahedron. In other words, c is the distance from the center $S\ \left[\frac{\sqrt{6}}{3}c, \frac{\sqrt{2}}{3}c, \frac{c}{3}\right]$ of this sphere to any vertex of tetrahedron structure of the carbon.

Conclusion

VFRT (vortex-fractal-ring theory) is a new and original view of elementary particles and the structure of atomic nuclei, atoms, and molecules. Its basics are simple for understanding through the comprehensive topological structure that does not need description by complicated mathematical formulas. This theory, based on the use of the vortex, fractal and ring structures, interconnects all the current knowledge. VFRT together with grammatical evolution can design new models of nanostructures. It allows us to understand the fundamental physical and chemical reasons for the stability and reactivity of atoms and molecules. Grammatical evolution is a suitable tool for optimizing the design of new nanostructures. This new way of designing nanostructures has been tested on the graphene structure. This article is an introduction to the problem of prediction of nanostructures using VFRT and grammatical evolution. The principle described in this article is not limited to structures that consist only of carbon atoms. It allows to design structures with different atoms in the near future. In the near future, the predicted structures will also use different atoms.

On **Fig. 7** is a comparison of classic spherical and new ring models **[10]**.

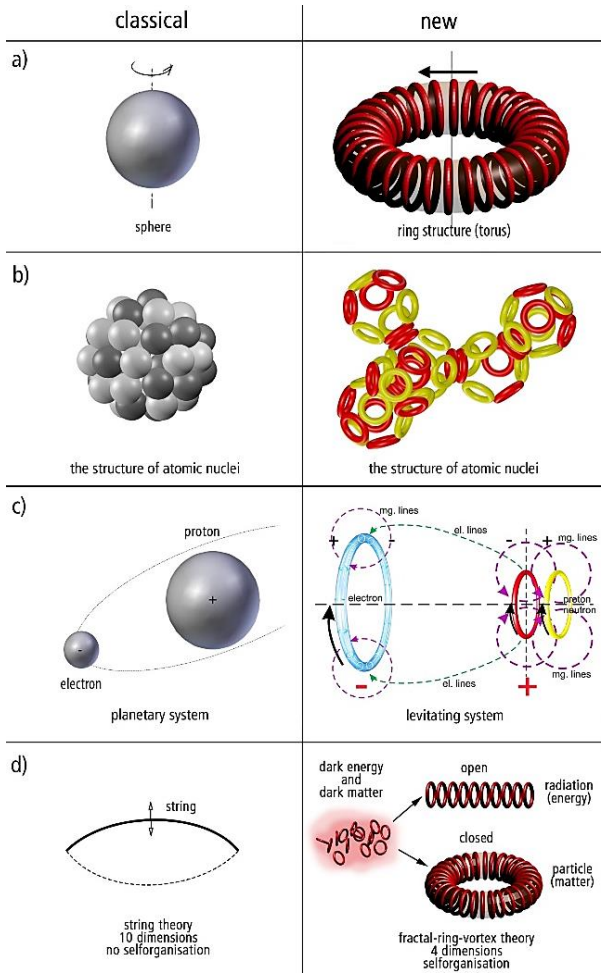

Fig. 7. Classic and new fractal ring models.

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12. More about VFRT can be found on http://www.pavelosmera.cz/public/public.html

