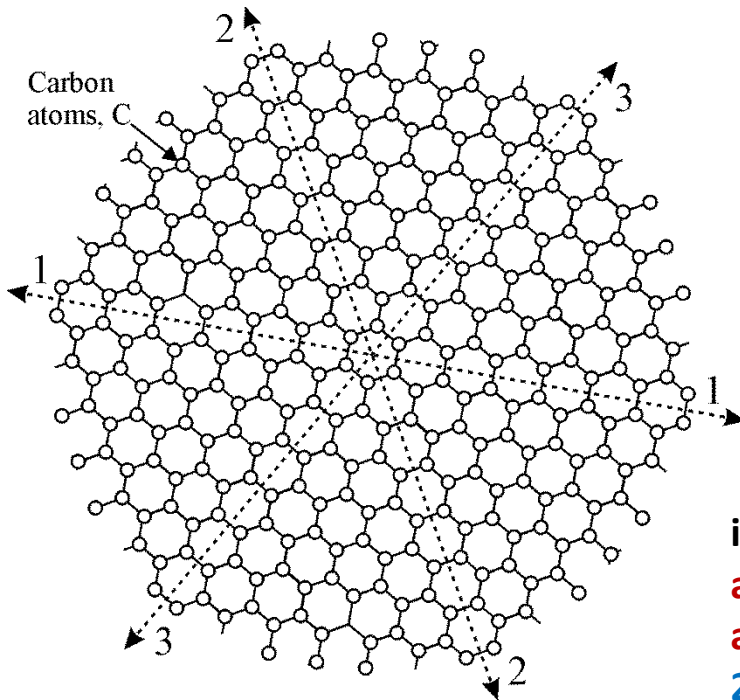# Anisotropy
of
Unstrained Pristine Graphene

(Discovery claimed in the application for a patent EP2401764
Priority date 24.02.2009)

George Shpenkov

http://shpenkov.com/pdf/talk2016Paris.pdf

Conventional viewpoint on basic properties of Graphene

Carbon atoms, C

* [Robert E. Newnham, Properties of Materials: Anisotropy, Symmetry, Structure; Oxford University Press, 2005]

Graphene is an allotrope of carbon in the form of a two-dimensional hexagonal lattice.

Point group D6h, space group P6/mmm

- **One atom** forms each node of the lattice.

- **sp² hybridized orbitals** are responsible for the bond of carbon atoms in the lattice.

- The lattice has **6-Fold** rotational symmetry.

Hence,

in full agreement with the **basic symmetry theory***, **all properties,** including electronic conductivity, along the **crystallographically identical** directions 1-1, 2-2, 3-3 (indicated here) **must be equal.**

However, our studies show that it is not true

Conventional view

is based (1) on an idea about the atom as having a superdense tiny nucleus and (2) on an idea about the electron configuration which is considered as responsible for interatomic bonds and, hence, for the structure of substances.

This is described within the Standard Model
in Quantum Mechanics (QM) and Quantum Chemistry (QC).

Whether these ideas are consistent with reality?

We have solid evidence to doubt in that. To the present we provided more than enough arguments proving fallibility of the QM and QC and their notions.

You can make sure in it,
if have a look at the publications as, for example, listed below:

L. Kreidik and G. Shpenkov, "*Important Results of Analyzing Foundations of Quantum Mechanics*", Galilean Electrodynamics & QED-East, Special Issues 2, 13, 23-30, (2002); http://shpenkov.com/pdf/QM-Analysis.pdf

G. Shpenkov and L. Kreidik, "*Schrodinger's Errors of Principle*", Galilean Electrodynamics, 3, 16, 51-56, (2005); http://shpenkov.com/pdf/blunders.pdf

G. P. Shpenkov, "*Conceptual Unfoundedness of Hybridization and the Nature of the Spherical Harmonics*", Hadronic Journal, Vol. 29. No. 4, p. 455, (2006); http://shpenkov.com/pdf/hybridizationshpenkov.pdf

G. P. Shpenkov, "*Some Words about Fundamental Problems of Physics*: *Constructive Analysis*", LAMBERT Academic Publishing, p.116 (2012); http://shpenkov.com/pdf/Book-2011-Eng.pdf

The actual situation in theoretical physics is so hopeless that there is an exceptional need in alternative theories that could take it out of stagnation. The present book offers the first real alternative to the bankrupt Standard Model. Basing on his long experience, the author has come to the conclusion that the current theoretical physics paradigm is erroneous and, therefore, must be changed. He has developed the Wave Model, physical, as an alternative to the abstract-mathematical Standard Model. The book differs by novel ideas. Along with the fair criticism, for all issues addressed in the book, clear solutions are presented. They were obtained on the basis of a new physics paradigm adequate to reality. In the literature on physics there is not a constructive analysis of fundamental problems of physics presented with such a manner as it is done in this book. Distinguishing features of the book are the breadth of issues covered by the analysis, its complexity and comprehensiveness, brevity and the use of simple and straightforward language. For this reason, the book will useful for all physicists, theorists and experimentalists, specialized in different branches of physics.

Dialectical physics paradigm

George Shpenkov

Some words about fundamental problems of physics

Constructive analysis

George Shpenkov

Comprehensive analysis of basic concepts of modern theoretical physics is presented in this book written in a concise and clear form. It is shown that the abstract-mathematical method dominated in theories of the Standard Model is erroneous and, therefore, dead-ended. The author proposes the real way to out of this situation.

Shpenkov

LAP LAMBERT
Academic Publishing

For many years research we were developing a

New Physics theory,

which could <u>solve the problems</u> unsolvable in principle
within the modern Standard Model (SM), even improved by String theories.

As a result we have created such a theory and called it the

Wave Model (WM)

It includes <u>Dynamic Model</u> of elementary particles and <u>Shell-Nodal</u> atomic model

New concepts,
formed in the WM on the basis of the discoveries,

about the *structure of atoms* and *their compounds*,

and on the *formation of intra-* and *interatomic bonds*,

<u>differ greatly</u>

from the corresponding concepts of the SM

It turned out that

Atoms

(except of one-nucleon hydrogen $^1_1$H) are the

elementary nucleon molecules

(without superdense tiny nuclei in their centres and in the centres of nucleons)

As a consequence of so fundamental discovery, **we have come to a series of other discoveries**. In particular, we found that

a two-dimensional hexagonal lattice of

Graphene,

made of the carbon elementary nucleon molecules ("atoms")

(having a unique molecular structure inherent just for carbon),

is

anisotropic

and has a

two-fold rotational symmetry

The Wave Model*

uses

I. *Dialectical logic,*

Unlike <u>formal logic</u> used by modern physics theories;

and is based on the <u>axiom</u> about

II. *The wave nature of all phenomena and objects in the Universe.*

– *This is one the <u>only axiom</u> lying in the foundation of the WM, and no postulates are used in the WM.*

– *While in the foundation of modern physics theories, there are **several dozen** of **abstract-mathematical (fictional)** <u>postulates</u>. The latter is the main reason of all the problems faced the Standard Model.*
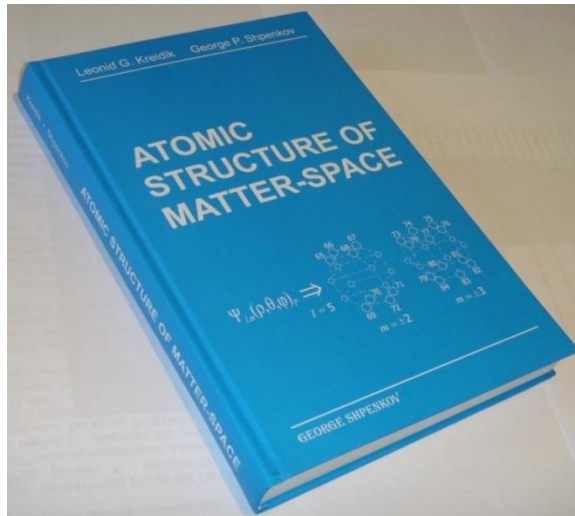
Revising the existent doubtful theoretical constructions, the Wave Model already resolved some of the problems unsolvable in principle within the SM.

The Wave Model
is described in detail in the book and lectures:

L. G. Kreidik and G. P. Shpenkov,
Atomic Structure of Matter-Space,
Geo. S., Bydgoszcz, 2001, 584 p.
http://shpenkov.com/atom.html

G. P. Shpenkov,
Dialectical View of the World:
The Wave Model
(Selected Lectures); Volumes 1-6

http://shpenkov.com/pdf/Vol.1.Dialectics.pdf
... /Vol.2.DynamicModel-1.pdf
... /Vol.3.DynamicModel-2.pdf
... /Vol.4.PhysicalUnits.pdf
... /Vol.5.Shell-NodalAtomicStructure.pdf
... /Vol.6.TopicalIssues.pdf

A new physics paradigm, lying in the base of the WM, led to a whole series of key discoveries collected in the Comparative Table*

*[G. P. Shpenkov, "***Conclusion***" in "***Some Words about Fundamental Problems of Physics: Constructive Analysis***", LAMBERT Academic Publishing, p.70-78 (2012)]
http://shpenkov.com/pdf/Conclusion-Eng.pdf

Major milestones

on the way to the discovery of

<div style="border: 2px solid gold; padding: 10px;">

Elementary Nucleon Molecules,
i.e., the Shell-Nodal structure of the "atoms"

</div>

and, as an effect, the discovery of

<div style="border: 2px solid gold; padding: 10px;">

Natural anisotropy
inherent to the hexagonal lattice of graphene

</div>

We took for granted that the **structure of atoms**, as all matter-space **having** (in accordance with the basic axiom of the WM) **the wave nature**, **must be described** by well-developed methods of the physics of waves and, in particular, by the
universal ("classical") wave equation

$$\Delta \hat{\Psi} - \frac{1}{c^2} \frac{\partial^2 \hat{\Psi}}{\partial t^2} = 0 \qquad (1)$$

Eq. (1) admits a **particular solution** of the form

$$\hat{\Psi}(\rho, \theta, \varphi; t) = \hat{\psi}(\rho, \theta, \varphi) e^{\pm i \omega t} \qquad (2)$$

which describes, as is well-known, <u>standing waves</u> in spherical space.

The **spatial component** in (2)

$$\hat{\psi}(\rho,\theta,\varphi) = A\hat{R}_l(\rho)\Theta_{l,m}(\theta)\hat{\Phi}_m(\varphi)$$
(3)

is a particular solution of the **time-independent form** of Eq. (1):

$$\Delta\hat{\psi} + k^2\hat{\psi} = 0$$
(4)

(called the **Helmholtz equation**).

The solution (3) defines:

The nodal structure of standing waves in spherical space
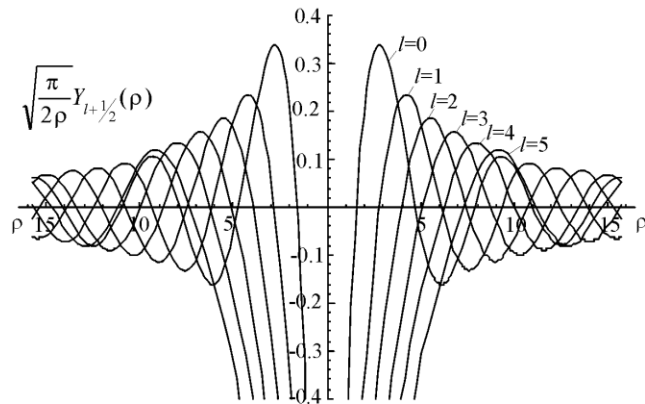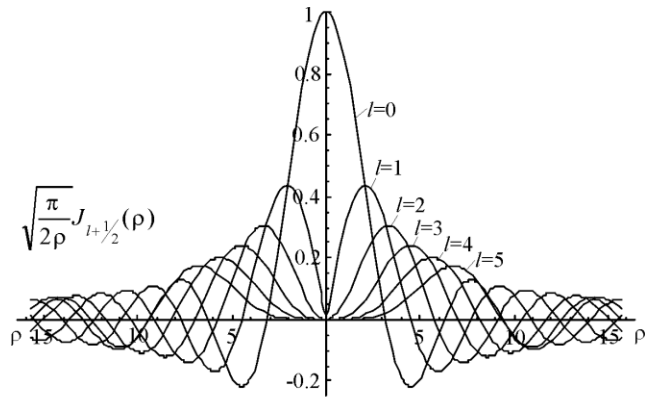
and, as we discovered, **defines also** the

Shell-Nodal structure of the atoms

which proven to be the

Elementary Nucleon Molecules!

- -

The wave vector $k = \omega_e/c$ is the constant. $\omega_e = 1.869162559\times10^{18}\ s^{-1}$
*is the **fundamental frequency** of the **atomic** and **subatomic** levels; $\rho = kr$*

Radial component $\hat{R}_l(\rho)$
of the solution $\hat{\psi} = A\hat{R}_l(\rho)\Theta_{l,m}(\theta)\hat{\Phi}_m(\varphi)$

$\sqrt{\dfrac{\pi}{2\rho}} J_{l+\frac{1}{2}}(\rho)$

$\sqrt{\dfrac{\pi}{2\rho}} Y_{l+\frac{1}{2}}(\rho)$

has the form:

$$\hat{R}_l(\rho) = A\sqrt{\pi/2\rho}\left(J_{l+\frac{1}{2}}(\rho) \pm iY_{l+\frac{1}{2}}(\rho)\right)$$

A is the constant factor;

$$l = 0,1,2,\ldots; \qquad m = 0,\pm 1,\pm 2,\ldots,\pm l$$

Solutions of $\hat{R}_l(\rho)$ are **roots** $z_{\nu,q}$ (zeros and extremal values) of **Bessel functions** J and Y, where $\nu = l + 1/2$ is the order of the functions , q is the number of the zero or extremum.

$\hat{R}_l(\rho)$ **defines the radii *r* of characteristic wave shells,** potential and kinetic on which are nodes and antinodes, respectively : $\rho_{\nu,q} = z_{\nu,q} = kr_{\nu,q}, \ \ k = \omega_e/c$.

Graphs of the polar functions

$$\left| \Theta_{l,m}(\theta) \right| = C_{l,m} \cdot P_{l,m}(\cos\theta)$$

$$P_{l,m}(\cos\theta) = \frac{\sin^m\theta}{2^l\, l!}\, \frac{d^{l+m}}{d(\cos\theta)^{l+m}}\left(\cos^2\theta - 1\right)^l$$

The adjoined Legendre functions

$m=0$ $m=1$ $m=2$ $m=3$ $m=4$ $m=5$

$l=1$ $l=2$ $l=3$ $l=4$ $l=5$

$\Theta_{l,m}(\theta)$
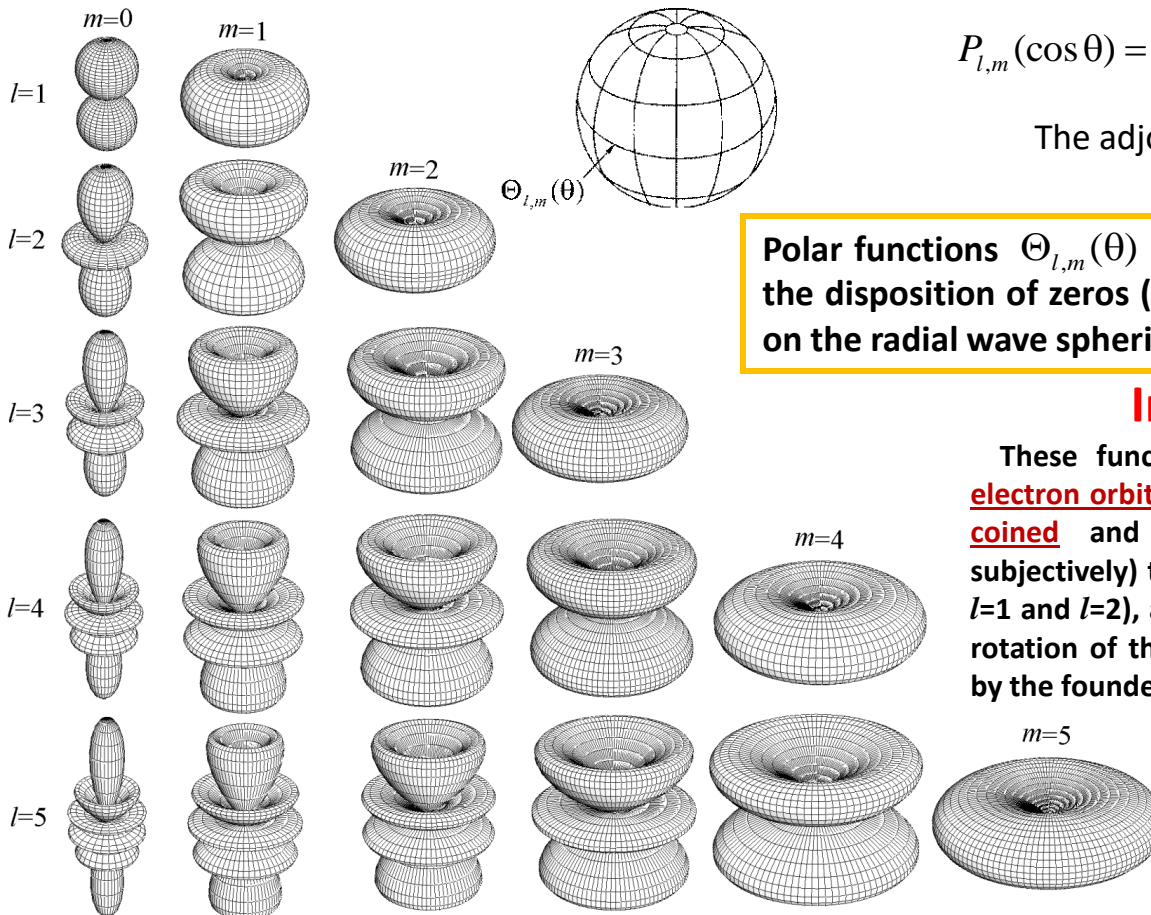
Polar functions $\Theta_{l,m}(\theta)$ **define characteristic parallels of the disposition of zeros (nodes) and extremes (antinodes) on the radial wave spherical shells.**

Important notice!

These functions <u>have nothing in common with electron orbitals.</u> The notion of <u>electron orbitals was coined</u> and attributed arbitrarily (unfoundedly, subjectively) to some of the functions $\Theta_{l,m}(\theta)$ (at l=1 and l=2), and to the spatial figures formed at the rotation of their sections, and combinations thereof by the founders of quantum mechanics.
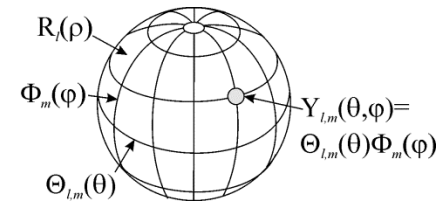
Graphs
of the polar-azimuthal functions

$$Y_{l,m}(\theta, \varphi)_p = \left| \Theta_{l,m}(\theta) Cosm\varphi \right|$$

(potential component)
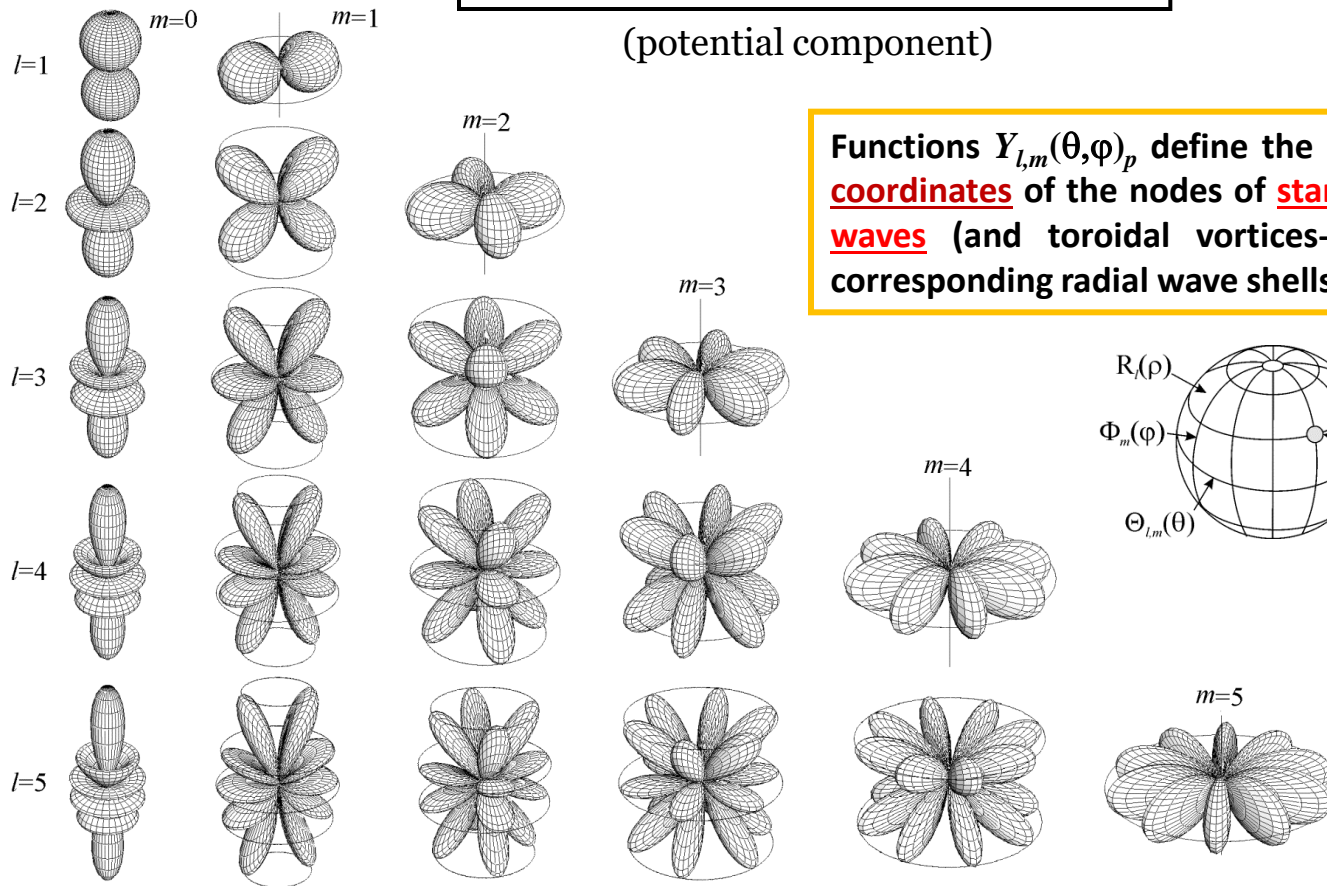
Functions $Y_{l,m}(\theta,\varphi)_p$ define the spatial **angular coordinates** of the nodes of **standing spherical waves** (and toroidal vortices-rings) on the corresponding radial wave shells.

The nodal structure
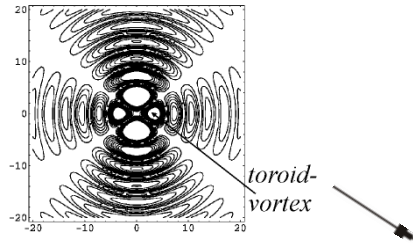# of standing waves in spherical space

The particular solution ψ_p of the wave equation (1):

ψ_p is the potential component of $\hat{\psi}$

α is an initial phase of the azimuth state

$l = 0, 1, 2, \ldots \quad m = 0, \pm 1, \pm 2, \ldots, \pm l$

$$\psi_p = A\sqrt{\frac{\pi}{2\rho}} J_{l+\frac{1}{2}}(\rho)\Theta_{l,m}(\theta)Cos(m\varphi + \alpha)$$

Shells (l) and subshells (m)

The solution for $l = 2$, $m = 0$ (section $x = 0$)

toroid-vortex

This presentation of the solution (unknown earlier in physics) that we first made in 1980th **became key**. Just this image **led us** during lengthy comprehensive studies (the results of which were first published in 1996 [1]) to a **fundamental discovery** that this solution also **defines** the true **structure** of the **atoms** which really are the **Elementary Nucleon Molecules**

$\Theta_{5,2}(\theta)$ $Y_{5,2}(\theta,\varphi)$ $Y_{5,2}(\theta,\varphi)$ and $R_{5,2}(r_0)$

$l=5$
$m=\pm 2$
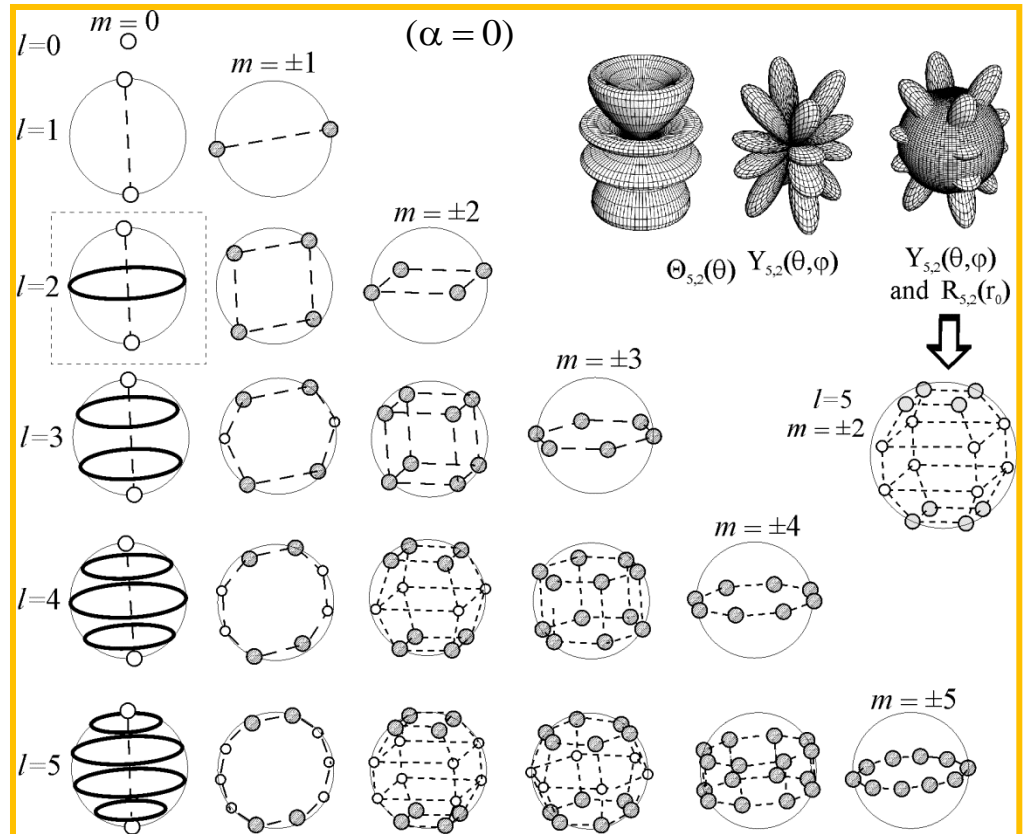
How we unraveled this mystery?
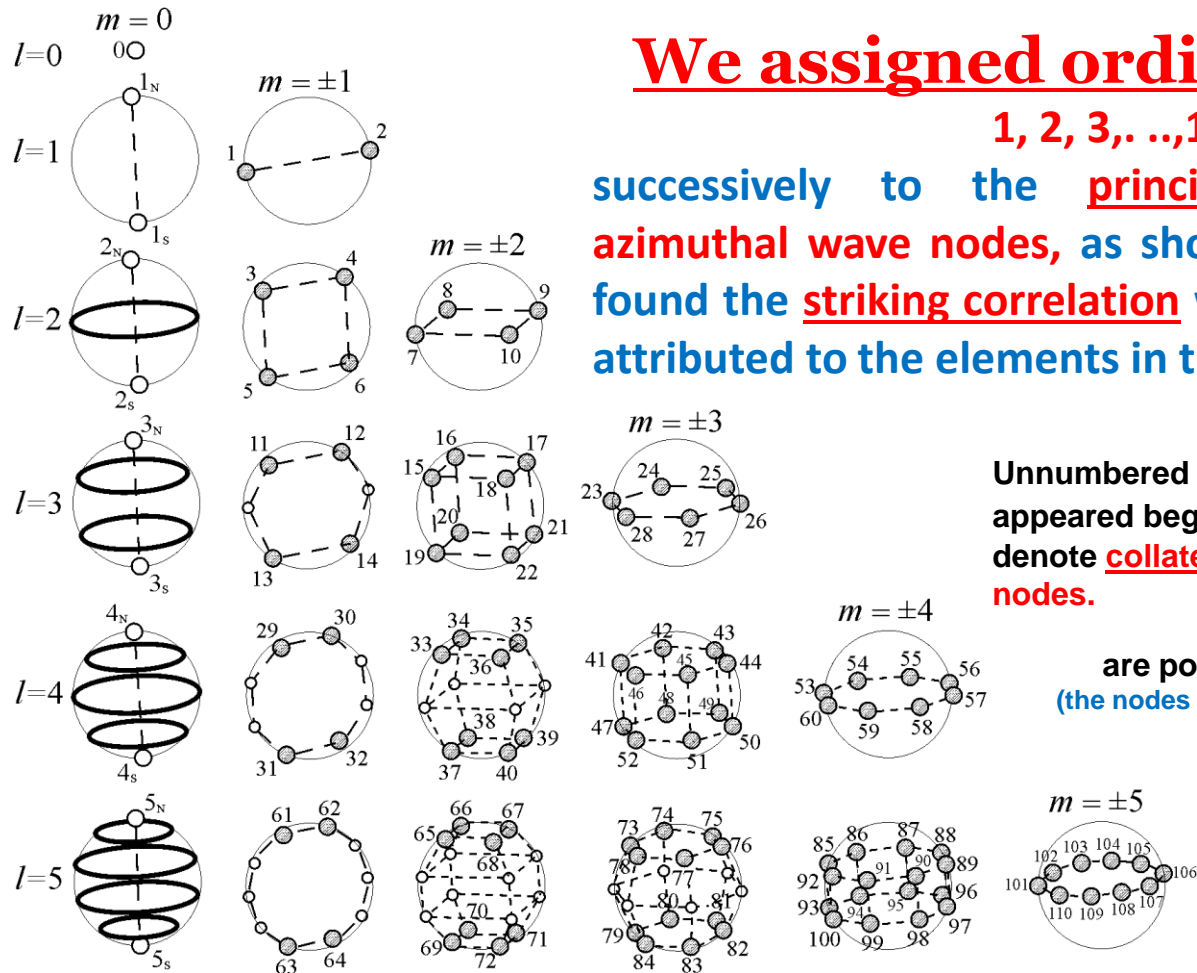
We assigned ordinal numbers
1, 2, 3,. ..,110

successively to the **principal** potential polar-azimuthal wave nodes, as shown in this figure, and found the **striking correlation** with **atomic numbers** Z attributed to the elements in the **Periodic Table**.

Unnumbered small empty circles (○), appeared beginning from $l = 3, m = \pm 1$, denote **collateral** potential polar-azimuthal nodes.

0, 1_N, 1_S,…, 5_N, 5_S
are potential-kinetic polar nodes
(the nodes of rest and motion simultaneously)

Analyzing further characteristic features of the solutions, presented in this way with the numbered nodes, we made sure, ultimately, that they really give us information about the true structure (shell-nodal) of the "atoms" which, in fact, are the elementary nucleon molecules [1, 2].

Elementary nucleon molecules

("atoms") having the
## fully completed and half-completed
outer wave shells
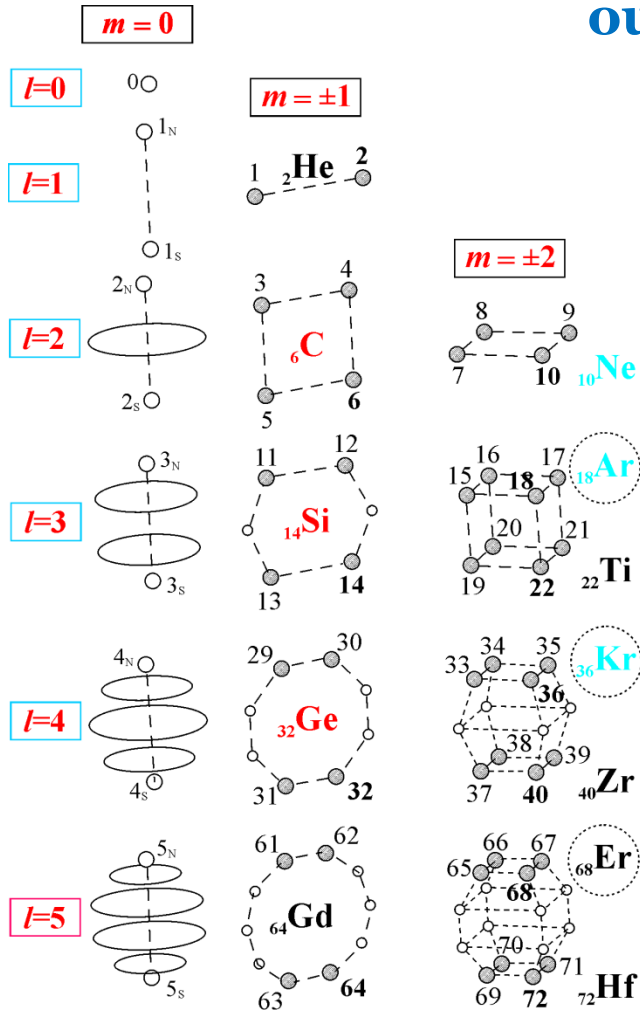
Half-integer outer shells have (according to the noninteger solutions) such "atoms" as, e.g., $_{18}Ar$, $_{36}Kr$, $_{68}Er$, $_{46}Pd$, $_{78}Pt$, $_{92}U$ (indicated in the intermittent circles)

Each of the principal potential polar-azimuthal nodes is filled with 2 hydrogen atoms, to which we refer proton, neutron, and protium.

For example, $_2He$ has in two such nodes (numbered 1 and 2) 4 hydrogen atoms (2x2).

$_6C$ has in 6 nodes (numbered 1, 2, and 3, 4, 5, 6) on two its shells (internal and external) 12 hydrogen atoms (6x2).
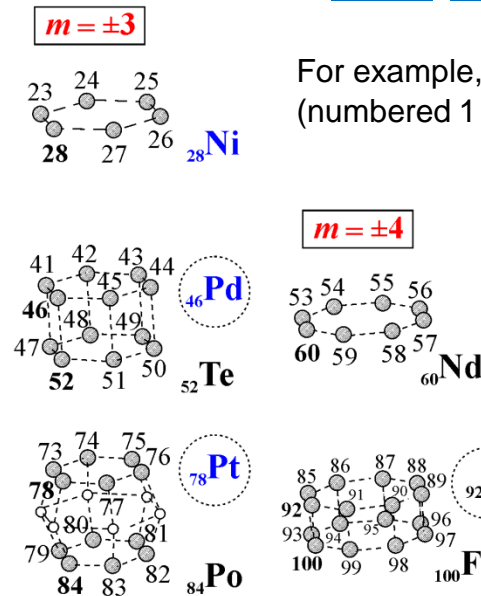
Noninteger solutions

$$l = m = s/2, \quad s \in \mathbf{N},$$

correspond to **intermediate states.** They define uncompleted external shells and subshells: **half-filled** (shown above) and **partially filled**, such as the shells of $_3$**Li,** $_4$**Be,** $_5$**B** or $_7$**N,** $_8$**O,** $_9$**F,** etc.

$$\hat{\psi} = A\sqrt{\frac{\pi}{2\rho}}\left(J_{\frac{s}{2}+\frac{1}{2}}(\rho) \pm iY_{\frac{s}{2}+\frac{1}{2}}(\rho) \right)\sin^{\frac{s}{2}}\theta\left(\cos\frac{s}{2}\varphi \pm i\sin\frac{s}{2}\varphi\right)$$
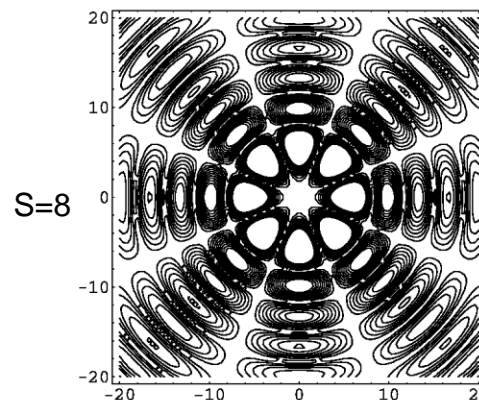
Zeros and extremes of the **noninteger solutions** (nodes and antinodes) are in the **equatorial plane** (z=0); they have **any-fold symmetry**, including <u>**forbidden by mathematical laws of crystallography**</u>. Here are two examples.

Contour plots of the sections for the potential component of the solutions, determined by the function $\boxed{\dfrac{J_{\frac{s}{2}+\frac{1}{2}}(\rho)}{\sqrt{\rho}}\sin^{\frac{s}{2}}\theta\cos\left(\frac{s}{2}\varphi\right)}$
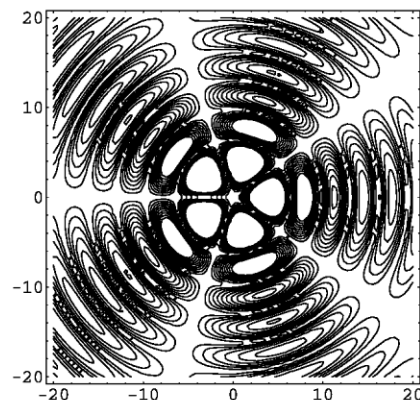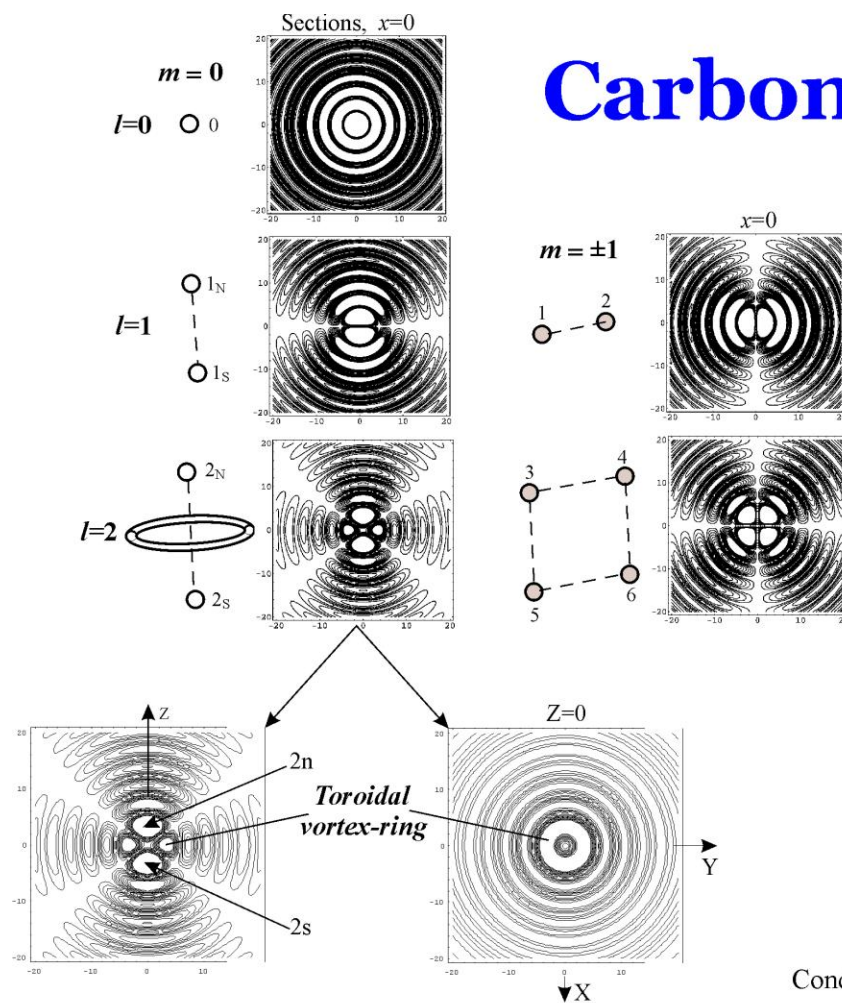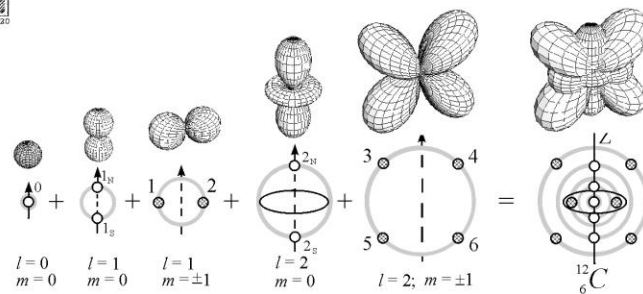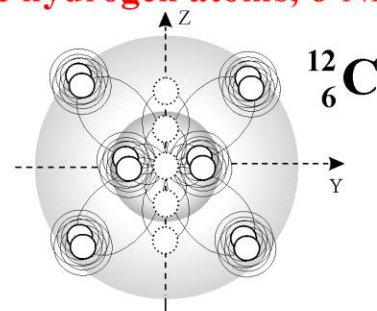

S=5   S=8

An equatorial distribution of the nodes of the **five-** and **eight-fold symmetries**

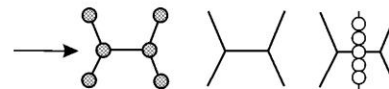# Shell-Nodal Structure of the Carbon Elementary Nucleon Molecule
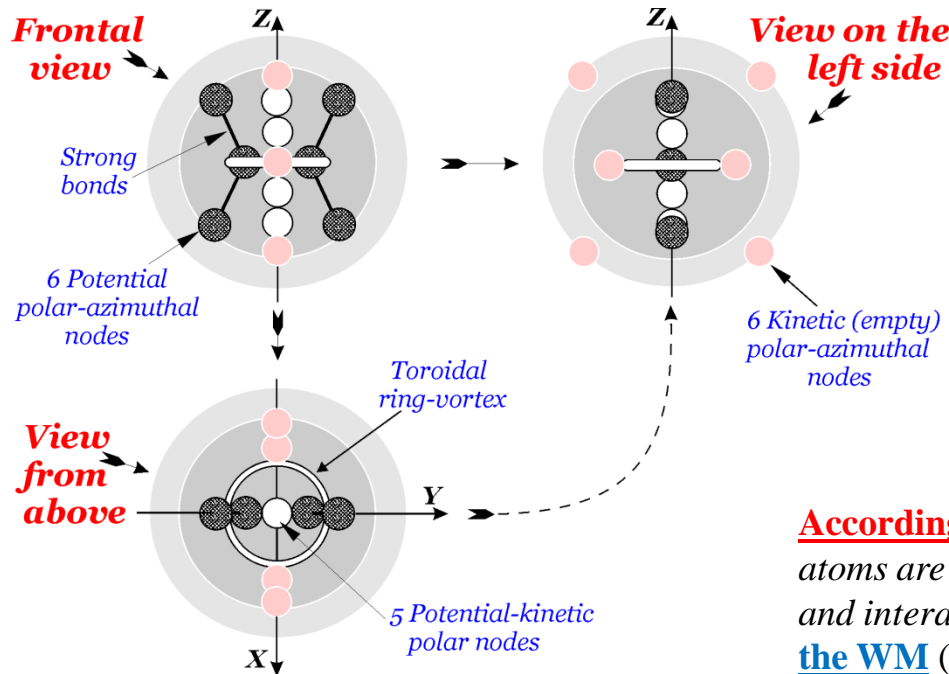

Carbon "Atom"

Six-nodal elementary molecule of the hydrogen atoms, 6-NEM

$^{12}_{6}C$

Carbon Elementary Nucleon Molecule (carbon "atom") $_6C$

Frontal view

Strong bonds

6 Potential polar-azimuthal nodes

View from above

Toroidal ring-vortex

5 Potential-kinetic polar nodes

View on the left side

6 Kinetic (empty) polar-azimuthal nodes

Potential and **kinetic** polar-azimuthal nodes are shifted relatively each other in radial direction, and lie in the planes, differing in phase by $\varphi = \pi/2$

Fundamental frequency and the fundamental wave radius of the atomic and subatomic levels:

$$\omega_e = 1.869162559 \times 10^{18}\ s^{-1}$$

$$\lambdabar_e = \frac{c}{\omega_e} = 1.603886492 \times 10^{-8}\ cm$$

According to the WM, *all elementary particles and atoms are **dynamic spherical formations** pulsating and interacting at the frequency* ω_e **discovered in the WM** (*along with* ω_g *and* E_B).

Binding energy *of the nodes in* $^{12}_{6}C^{-4}$, *calculated by*

the formula $\boxed{E_B = \omega_e^2\, \frac{m_1 m_2}{8\pi \varepsilon_0 r}}$, is $E_{C,ion} = 92.349...\,\text{MeV}$

$\omega_e m_2 = q_1$ *and* $\omega_e m_1 = q_1$ *are **exchange charges of** interacting nucleons;* $\varepsilon_0 = 1\,g \cdot cm^{-3}$ *is the **absolute unit density***

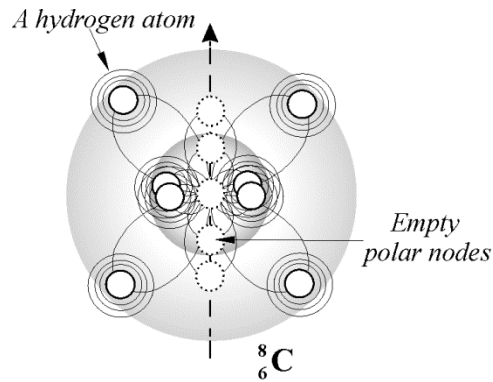*Fundamental frequency and the fundamental wave radius of the gravitational level:*

$$\omega_g = 9.158082264 \times 10^{-4}\ s^{-1}$$

$$\lambdabar_g = \frac{c}{\omega_g} = 327.4 \times 10^{6}\ km$$
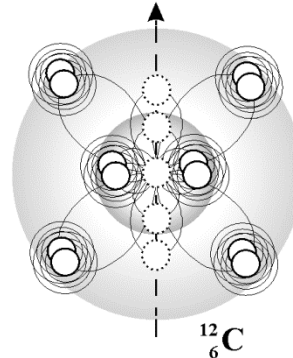
Thanks to the WM, the next mystery,

The nature of origin and the structure of all "atomic" isotopes,

was, at last, also unravelled.

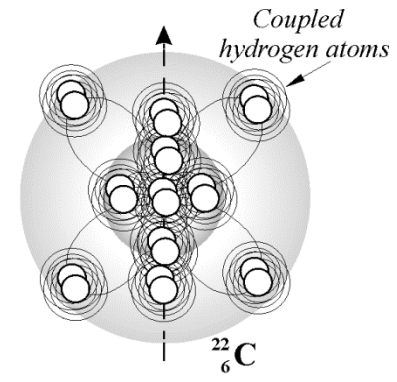## The stable and two limit short-lived isotopes of carbon*

A hydrogen atom

Empty polar nodes

$^{8}_{6}\text{C}$

The lightest isotope

(The least stable isotope with a half-life of 2.0×10^{-21} s)

$^{12}_{6}\text{C}$

The stable isotope

Coupled hydrogen atoms

$^{22}_{6}\text{C}$

The heaviest isotope

(A half-life of 6.2×10^{-3} s)

*[G. P. Shpenkov, *Physics and Chemistry of Carbon in the Light of Shell-Nodal Atomic Model*, Chapter 12 in "*Quantum Frontiers of Atoms and Molecules*", edited by Putz M. V., NOVA SCIENCE PUBLISHERS, NY, 277-323, 2011]
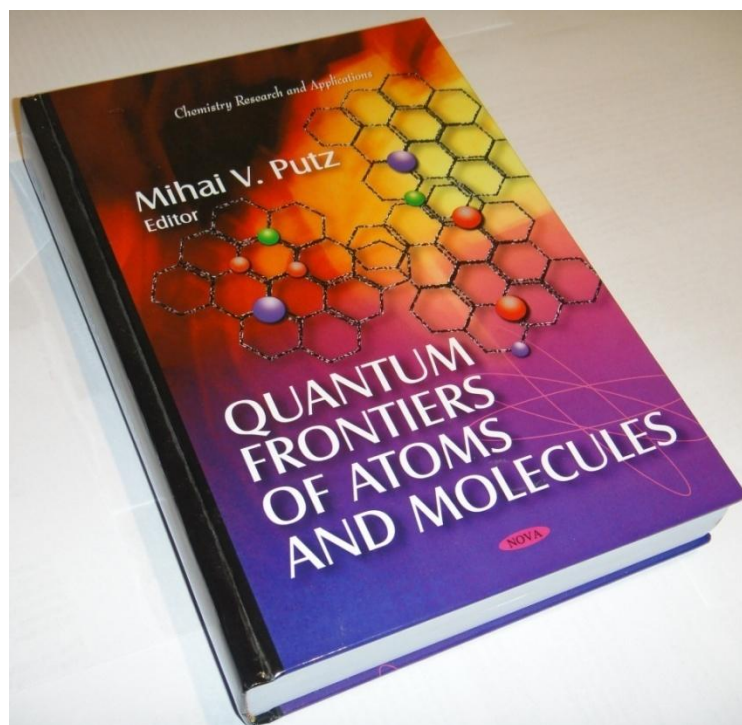
This is another in a series of the discoveries following from the fundamental discovery (the shell-nodal structure of the "atoms") and, thereby, directly confirming reality of the latter

The Complete Set of "Atomic" Isotopes

(Isotopes of elementary nucleon molecules)

natural and artificial, already detected and not yet detected.
Their number is limited in Nature by the given set, that is conditioned by the limited number of the combinations in filling the nodes (except of kinetic).

Particular solutions of the wave equation

$$\Delta\hat{\psi} + k^2\hat{\psi} = 0$$

The *left* and *right* boundaries indicate the *minimal* (for atoms with integer shells) and *maximal* (for all atoms) possible values of relative masses
(Atoms with *half-integer* external shells can have more isotopes of the *less minimal* masses then indicated here)

Stable and *long-lived* ($2.0 \times 10^5 < \tau < 1.4 \times 10^{10}$ y) isotopes

The nodal structure of the lightest 6-C-8, stable 6-C-12, and heaviest 6-C-22 isotopes of carbon

Hydrogen atoms: proton, neutron, and protium

Atomic number, Z
(the number of principal potential polar-azimuth nodes)

$Z = \sum_i Z_{gi}$

$A = \sum_k Z_{pk}\eta_{pk} + \sum_i (Z_{gi}\eta_{gi} + Z_{vi}\eta_{vi})$

(k and i are numbers of polar and polar-azimuth shells, respectively; Z_{pk} is the number of polar nodes of k-th polar shell; Z_{gi} and Z_{vi} are the number of principal and collateral polar-azimuth nodes, respectively, of i-th polar-azimuth shell; η_{pk}, η_{gi} and η_{vi} are numbers of multiplicity of the corresponding nodes, equal to zero, one or two)

Relative mass, A
(the number of hydrogen atoms in the nodes of the rest "atoms")

G. P. Shpenkov, **Physics and Chemistry of Carbon in the Light of Shell-Nodal Atomic Model**, Chapter 12 in **"Quantum Frontiers of Atoms and Molecules"**, edited by Putz M. V., NOVA SCIENCE PUBLISHERS, NY, 277-323, 2011.


A colour variant of the **Table of Isotopes** of 2001
is available online at **http://shpenkov.com/pdf/isotopes.pdf**

Periodic Table of the "Atoms"
(Elementary Molecules of the Hydrogen Atoms*)

{1, 2, 3, 4, ...} = Z are numbers of the principal potential polar-azimuthal nodes in the wave shells of the "atoms" ("Atomic" number)

Numbers of the nodes ("Atomic" numbers Z)

Principal potential polar-azimuthal nodes

Collateral potential polar-azimuth nodes (unnumbered)

Particular time-independent solutions of Eq.

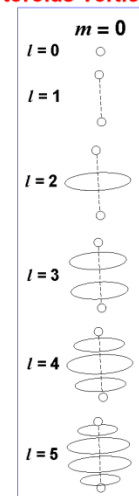$$\Delta\hat{\Psi} - \frac{1}{c^2}\frac{\partial^2\hat{\Psi}}{\partial t^2} = 0$$
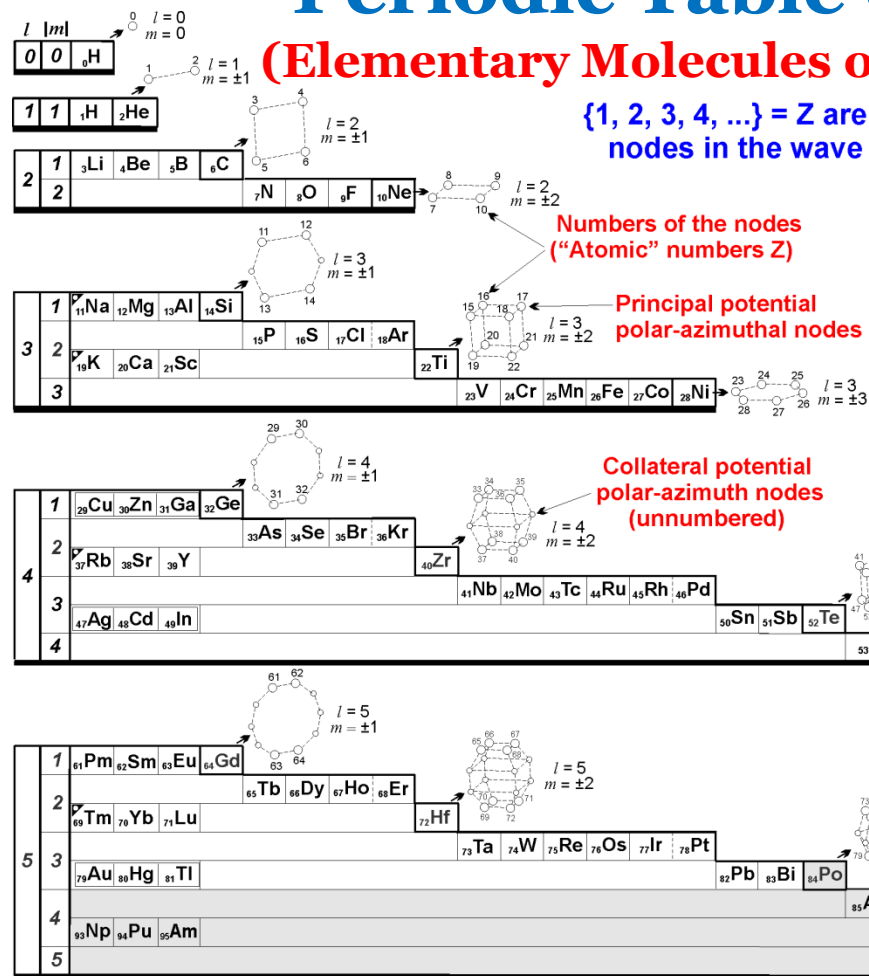
Atoms with completely filled external wave shells

$_2$He			
$_6$C	$_{10}$Ne		
$_{14}$Si	$_{22}$Ti	$_{28}$Ni	
$_{32}$Ge	$_{40}$Zr	$_{52}$Te	$_{60}$Nd
$_{64}$Gd	$_{72}$Hf	$_{84}$Po	$_{100}$Fm $_{110}$Ds

▨ ← **unstable elements**

Polar nodes and toroids-vortices

$m = 0$
$l = 0$
$l = 1$
$l = 2$
$l = 3$
$l = 4$
$l = 5$

[1] *Alternative Picture of the World*, V. 1-3, (1996); [2] *Foundations of Physics*, (1998);
[3] *Atomic Structure of Matter-Space*, (2001); Geo. S., Bydgoszcz by L. Kreidik and G. Shpenkov.
The Shell Structure of Matter Spaces, http://shpenkov.janmax.com/ShellStr.pdf

Copyright © 2001, 2016 George P. Shpenkov

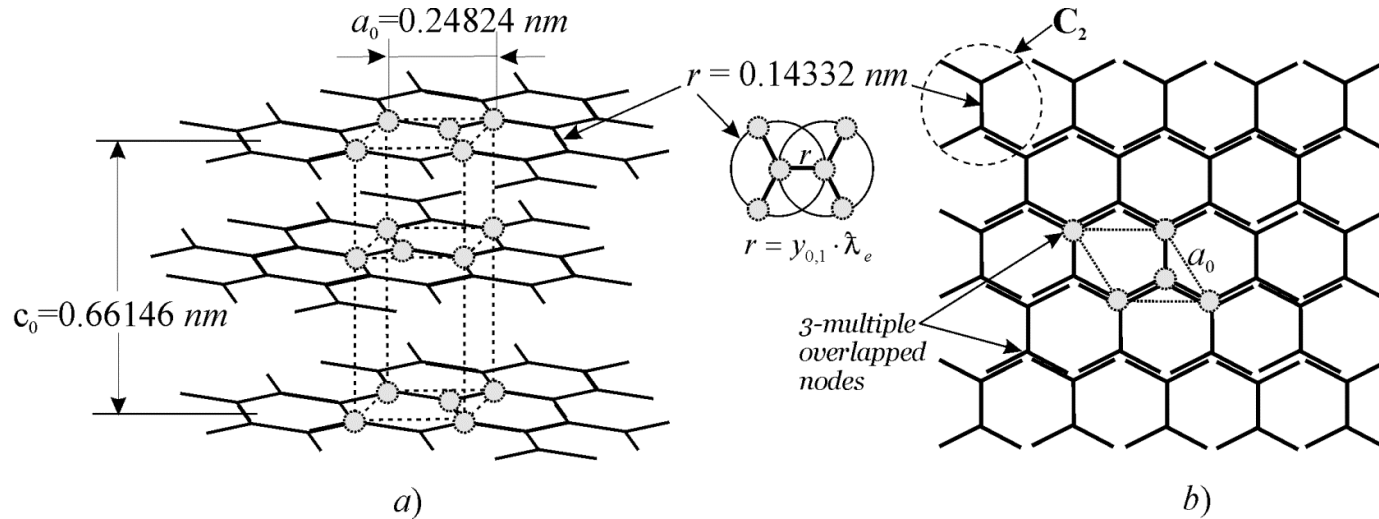***** **The hydrogen atoms:**
proton, neutron, and protium

Thanks to the solutions, it is revealed now the primordial true cause of the observable similarity in properties of the elements, first generalized and established by D. I. Mendeleev for chemical properties as the Law of Periodicity.

G. P. Shpenkov, **An Elucidation of the Nature of the Periodic Law**, Chapter 7 in **"The Mathematics of the Periodic Table"**, edited by Rouvray D. H. and King R. B., NOVA SCIENCE PUBLISHERS, NY, 119-160, 2006.
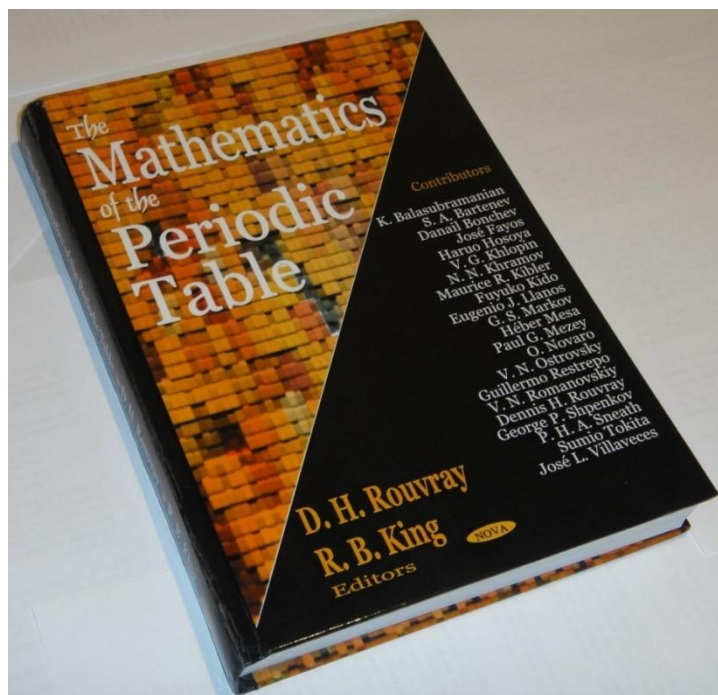
A colour variant of the **Periodic Table** of 2001
is available online at **http://shpenkov.com/pdf/placard.pdf**

A unit cell and the structure of graphite and its single atomic layer – graphene

$a_0 = 0.24824\ nm$

$r = 0.14332\ nm$

C_2

$r = y_{0,1} \cdot \tilde{\lambda}_e$

$c_0 = 0.66146\ nm$

3-multiple overlapped nodes

a_0

a)   b)

According to the WM, the **bonds length** in graphite is defined by the product $\boxed{r = y_{0,1} \cdot \tilde{\lambda}_e}$, **where** $y_{0,1}$ **is the root of Bessel functions [3]** $(y_{0,1}=0.89357697)$ **and** $\tilde{\lambda}_e = \omega_e / c = 1.603886538 \cdot 10^{-8}\ cm$

$$n = (1\tfrac{1}{6} \times 2 + 1\tfrac{2}{3}) = 4\ nodes\ per\ unit\ cell,\ V = n \cdot 12.0107 \cdot m_u / \rho = 35.29953318 \cdot 10^{-24}\ cm^3,$$
$$m_u = 1.660539040 \cdot 10^{-24}\ g,\ \rho = 2.26\ g \cdot cm^{-3},\ a_0 = \sqrt{3}r,\ c_0 = V \cdot 2 / a_0^2 \sqrt{3} = 6.614634572 \cdot 10^{-8}\ cm$$

Lattice constants a_o and c_o, calculated as shown here, are close to the lattice constants of graphite (at 300 K) known from the literature. The calculation data correspond to graphite consisting of <u>carbon dimers</u> C_2 having the shell-nodal structure.

Thus, we have come to the conclusion that the "building blocks" of graphite and, hence, graphene are carbon dimers C_2.

Precise calculations of atomic positions and the length of interatomic bonds

*are based on an **iterative method**: by **comparison** and **fitting** of measured intensities of a reflected beam with calculated, **taking into account Rutherford-Bohr's nuclear model of atoms**, so as long as will not be achieved an adequate correspondence of two sets of the values.*

*In accordance with the WM, we should take into account, at the iteration, the **shell-nodal** (molecule-like) **atomic model**.*

*Under this condition, calculation results of **lattice constants** for graphite will coincide practically with the known data, within the error limits, if only we will take **the dimer (C_2) of carbon elementary nucleon molecule** as an elementary "building block" of graphite, but not the elementary molecule (C) (i.e. **not the carbon "atom"**).*

This conclusion relates also to various other carbon compounds.

(In further discussion, we will adhere of this)

Schematic showing
the formation of the C$_2$ molecule

C$_2$ is forming by overlapping, "confluence", of all approaching nodes (and toroidal rings-vortex, not shown here) of two carbon nucleon molecules ("atoms") in the unit whole.

Like as magnets, two carbon "atoms" are attracted to each other by opposite directed fields of their internal internodal bonds

$$\mathbb{C} + \mathbb{C} \longrightarrow \mathbb{C}_2$$
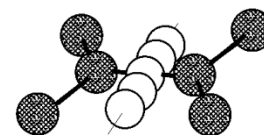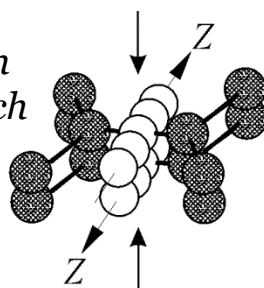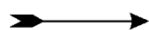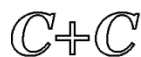
Conditional designations of the carbon "atom" C and the molecule C$_2$ are the same
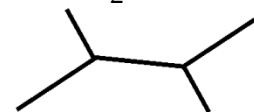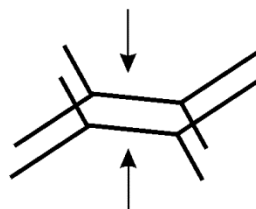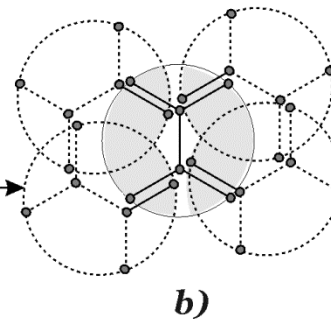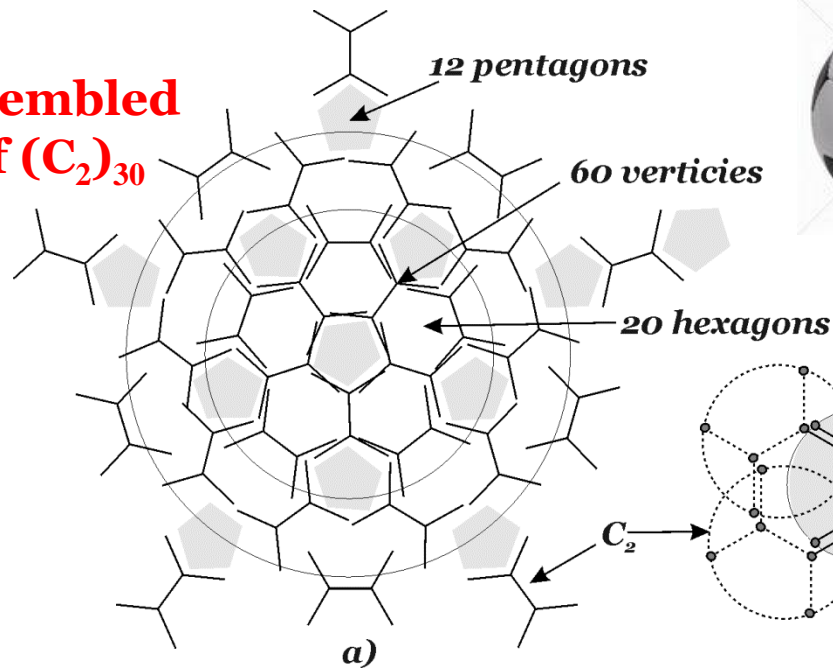
In [H. C. Shih, et al., *Diamond and Related Materials*, 2, 531 (1993)],

"...the C$_2$ radical was considered to be responsible for the formation of graphite"

In accordance with the WM,
Buckminsterfullerene (C_{60})
is formed of 30 carbon dimers C_2
and has the formula $(C_2)_{30}$

A disassembled view of $(C_2)_{30}$

12 pentagons

60 verticies

20 hexagons

C_2

Binding and overlapping of nodes

a)

b)

"Carbon Dimer (C_2) is in fact the major observable product of C_{60} fragmentation. Being a very effective growth species, it can rapidly incorporate into the diamond lattice leading to high-film growth rates"*.

*[D. M. Gruen, et al., Turning Soot Into Diamonds With Microwaves, Proceedings of the 29th Microwave Power Symposium, Chicago, Illinois, July 25-27, 1994]

A scheme showing
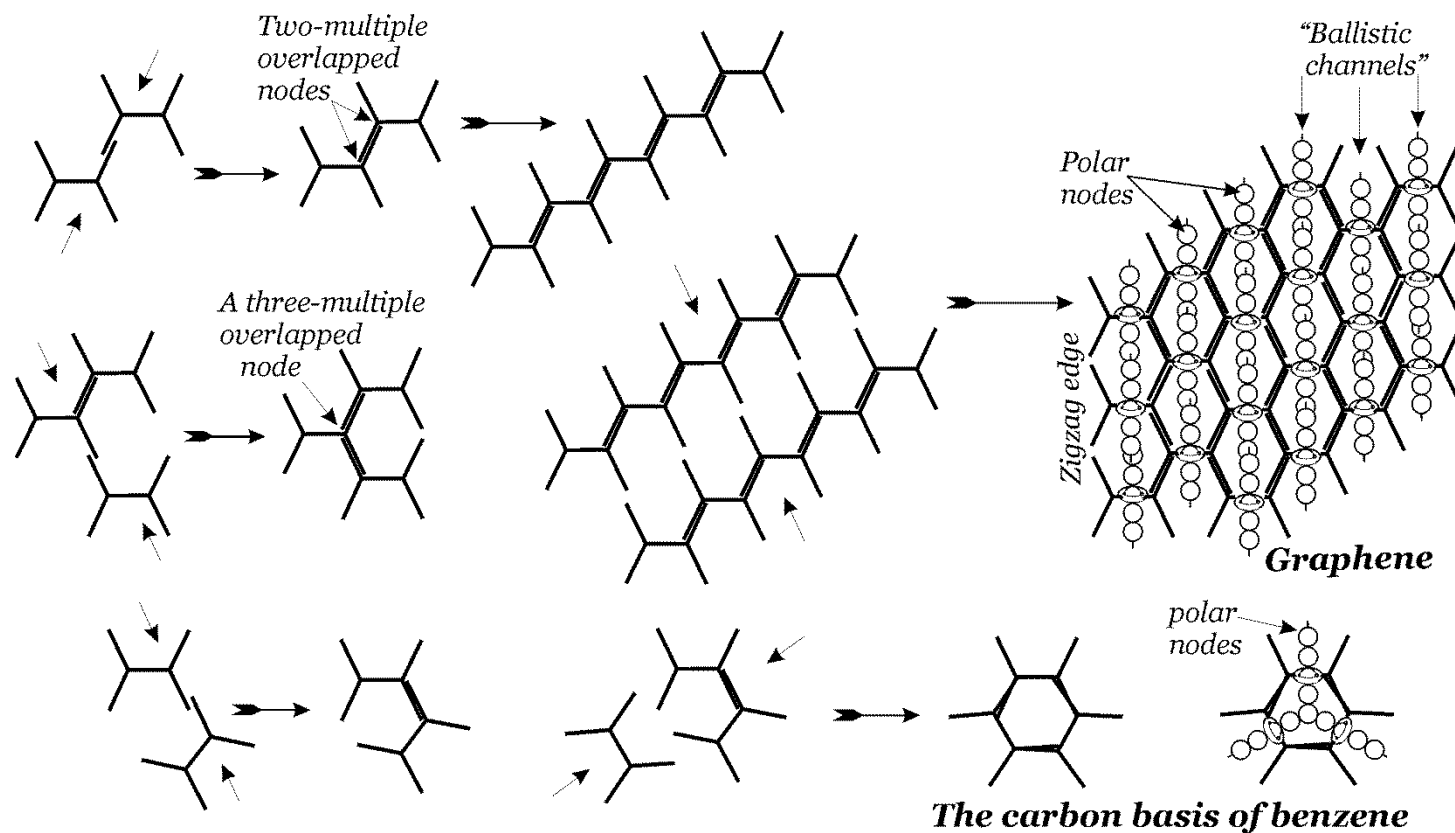# How chemical ("covalent") C−C bonds are formed
in hydrocarbon compounds

in ethane, C_2H_6 *in benzene*, $(C_2)_3H_6$
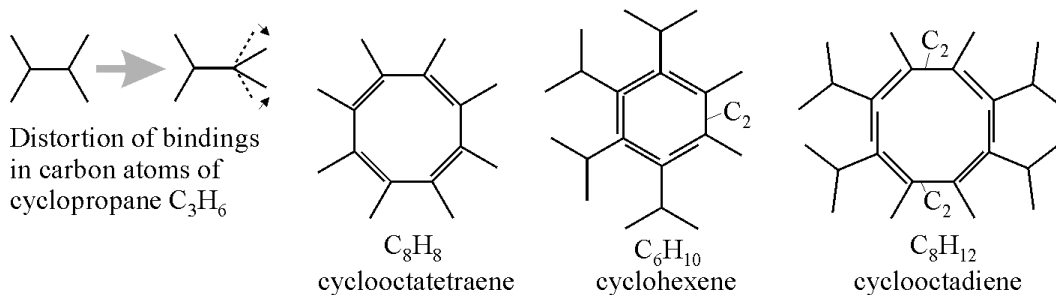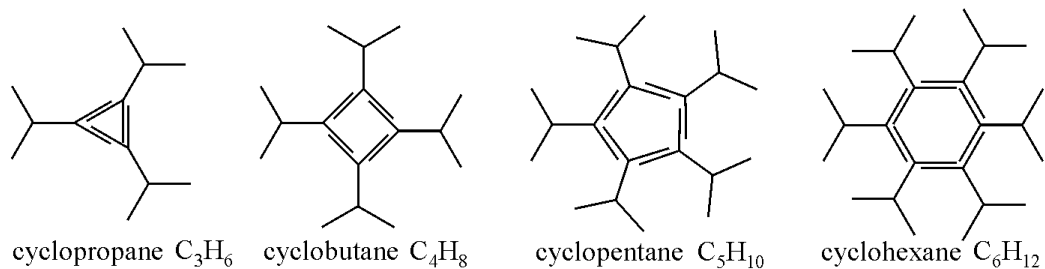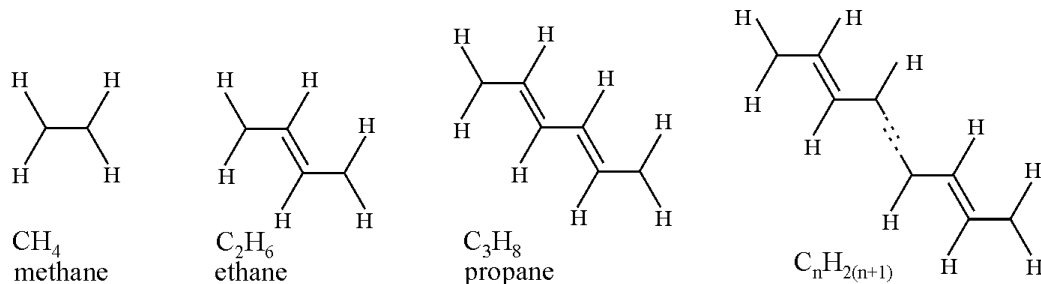
a)   *b)*   *c)*
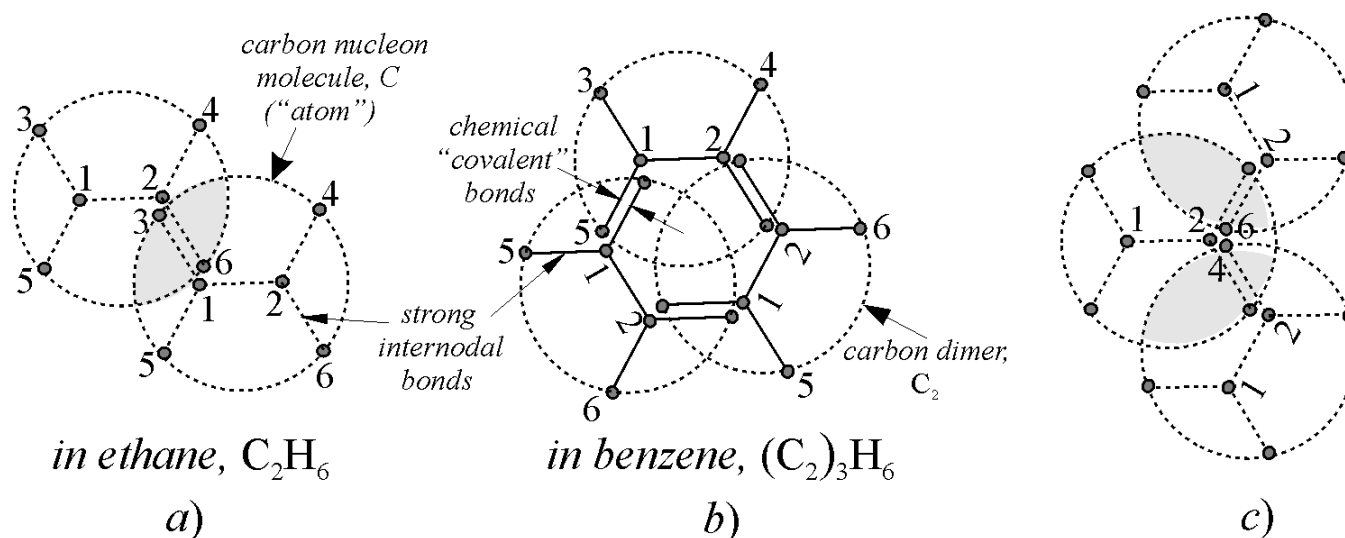
Two-multiple (a, b) and three-multiple (c) overlapping of polar-azimuthal nodes, external with internal, belonging to joined carbon nucleon molecules, single or dimmers.

Chemical "covalent" bonds are realized along the lines of strong internodal bindings (existing between external and internal nodes) each of the joined "atoms" (a) or dimers (b). Electrons play the secondary role because they define only the strength of the bonds.

# A schematic picture of self-binding (assembling) of 2D carbon compounds

Two-multiple overlapped nodes

A three-multiple overlapped node

Zigzag edge

"Ballistic channels"

Polar nodes

Graphene

polar nodes

The carbon basis of benzene

The structure of C-C bonds
in typical hydrocarbon compounds*

CH_4
methane

C_2H_6
ethane

C_3H_8
propane

$C_nH_{2(n+1)}$

cyclopropane C_3H_6 cyclobutane C_4H_8 cyclopentane C_5H_{10} cyclohexane C_6H_{12}

Distortion of bindings
in carbon atoms of
cyclopropane C_3H_6

C_8H_8
cyclooctatetraene

C_6H_{10}
cyclohexene

C_8H_{12}
cyclooctadiene

*[G. P. Shpenkov, *The Role of Electrons in Chemical Bonds Formations* (*In the Light of Shell-Nodal Atomic Model*), Molecular Physics Reports 41, 89-103, (2005)]

Formation of the internodal bonds in diamond

a)   *b)*   *c)*
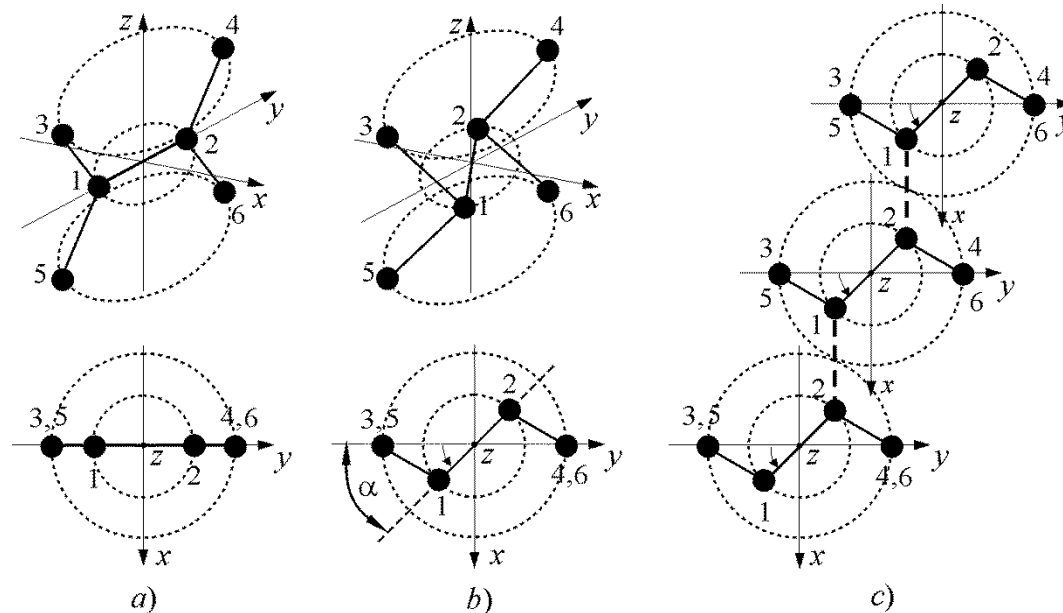
(a) *A plane structure of the **carbon dimer C$_2$** (and the **carbon "atom" C**).*

(b) *The turned position of the internal shell with nodes 1 and 2 with respect to the external shell by the **phase angle** $\alpha = \pi/4$ of the azimuth state that is **admitted by the solution** for φ, because* $\boxed{\Phi_p(\varphi) = \Phi_m \cos(m\varphi + \alpha)}$.

(c) **Bindings** *(dashed lines)* **between** *the turned* <u>**internal nodes 1 and 2**</u> *of the*

     nearby carbon dimmers, *resulted in a face-centered cube structure of diamond.*
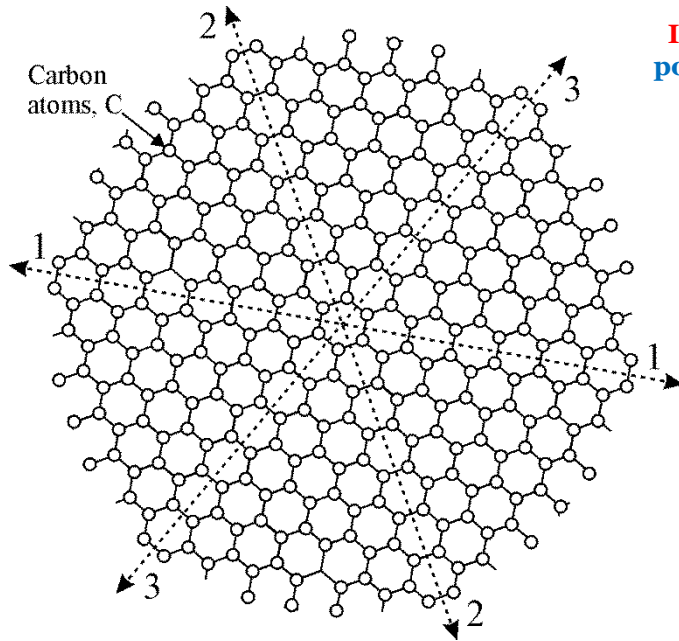
The face-centered cubic lattice of diamond

(made of carbon dimers C_2)

The overlap of the nodes

dimer C_2

tetrahedron

1.54 Å

a=0.3567 nm

a)   *b*)   *c*)   *d*)
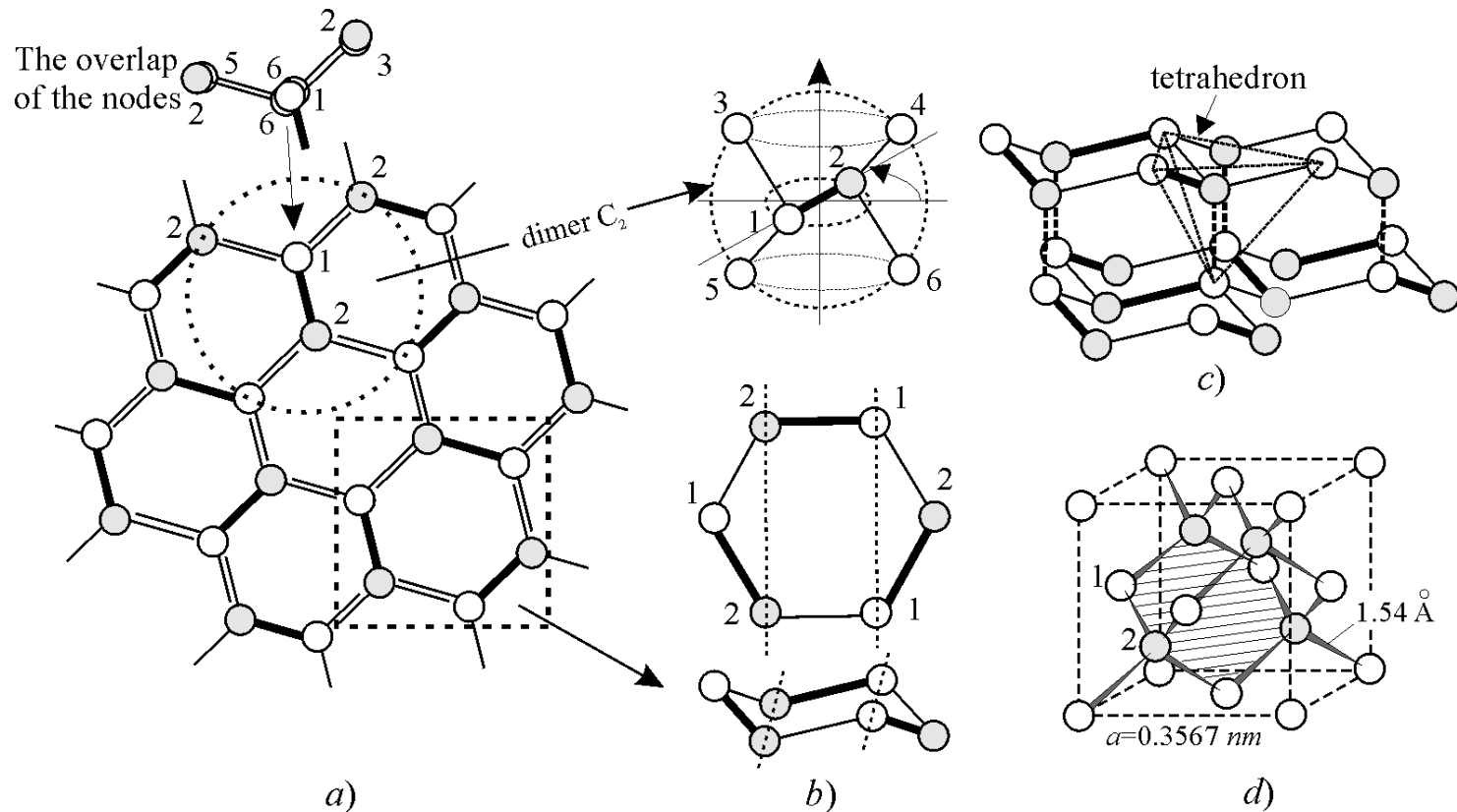
The Structure of Graphene

Conventional view

Hexagonal lattice is formed of <u>carbon atoms</u> C

Carbon atoms, C

6-fold
rotational symmetry

According to the WM

Hexagonal lattice is formed of <u>carbon dimers</u> C_2

Invisible polar potential-kinetic nodes

Carbon dimer C_2

Each polar-azimuthal node contains four hydrogen atoms

Each vertex of the lattice is formed of three overlapped nodes, belonging each to three bound carbon dimers C_2.
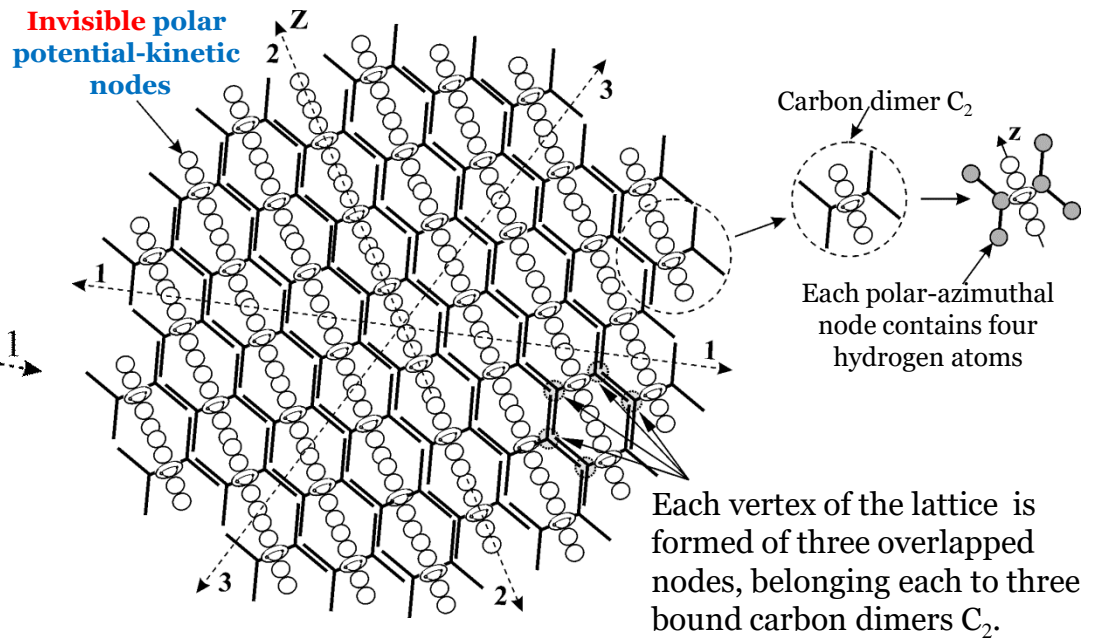
2-fold
rotational symmetry

An ordered "covalent" bond of carbon dimers C_2 is realized in graphene <u>along strong internodal bonds</u> in such a way that a continuous chain of empty polar nodes forms hollow channels inside the crystal, through which charge carriers can move without obstacles not being scattered, like it occurs at the **ballistic** motion.

The Edges in Graphene
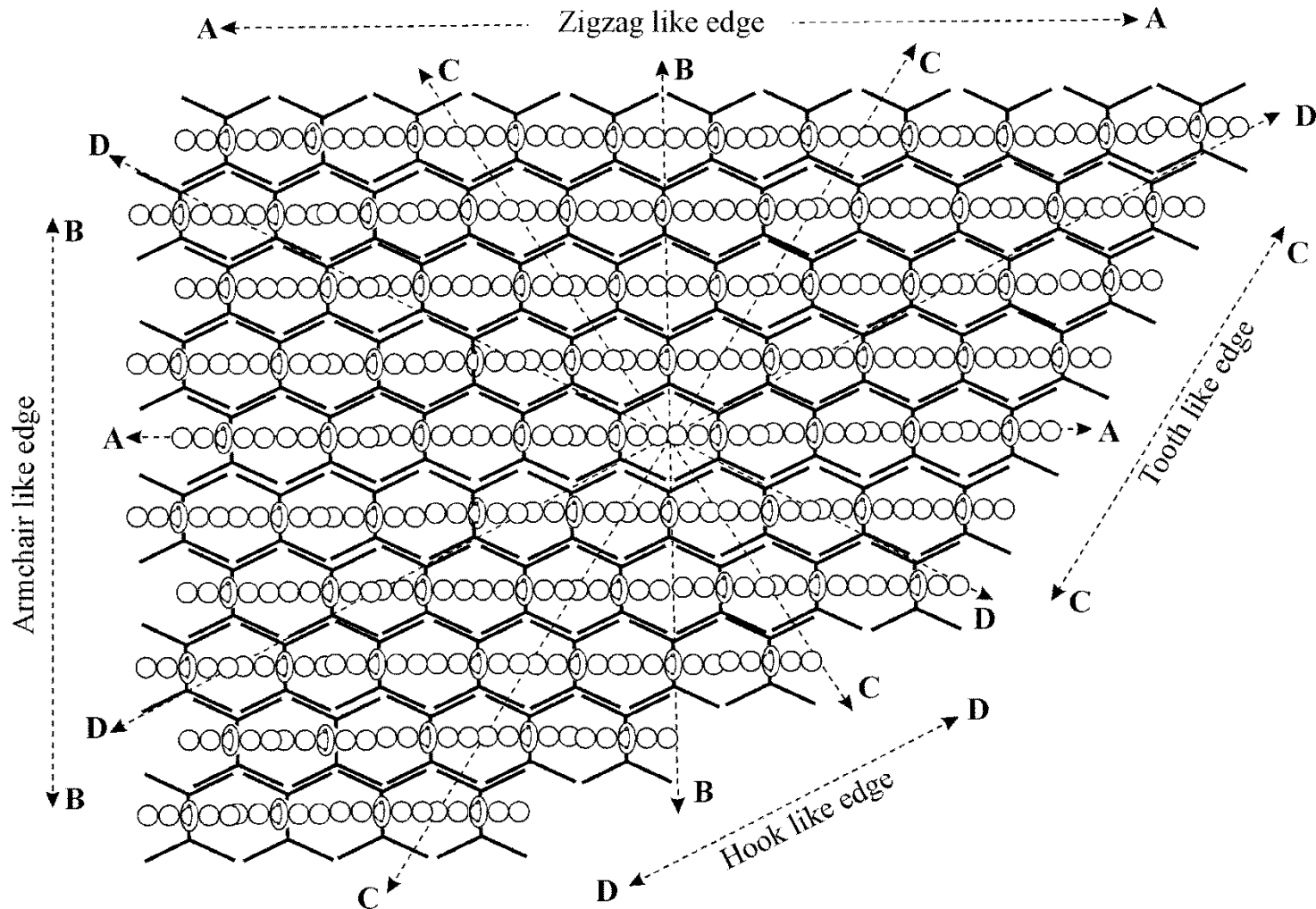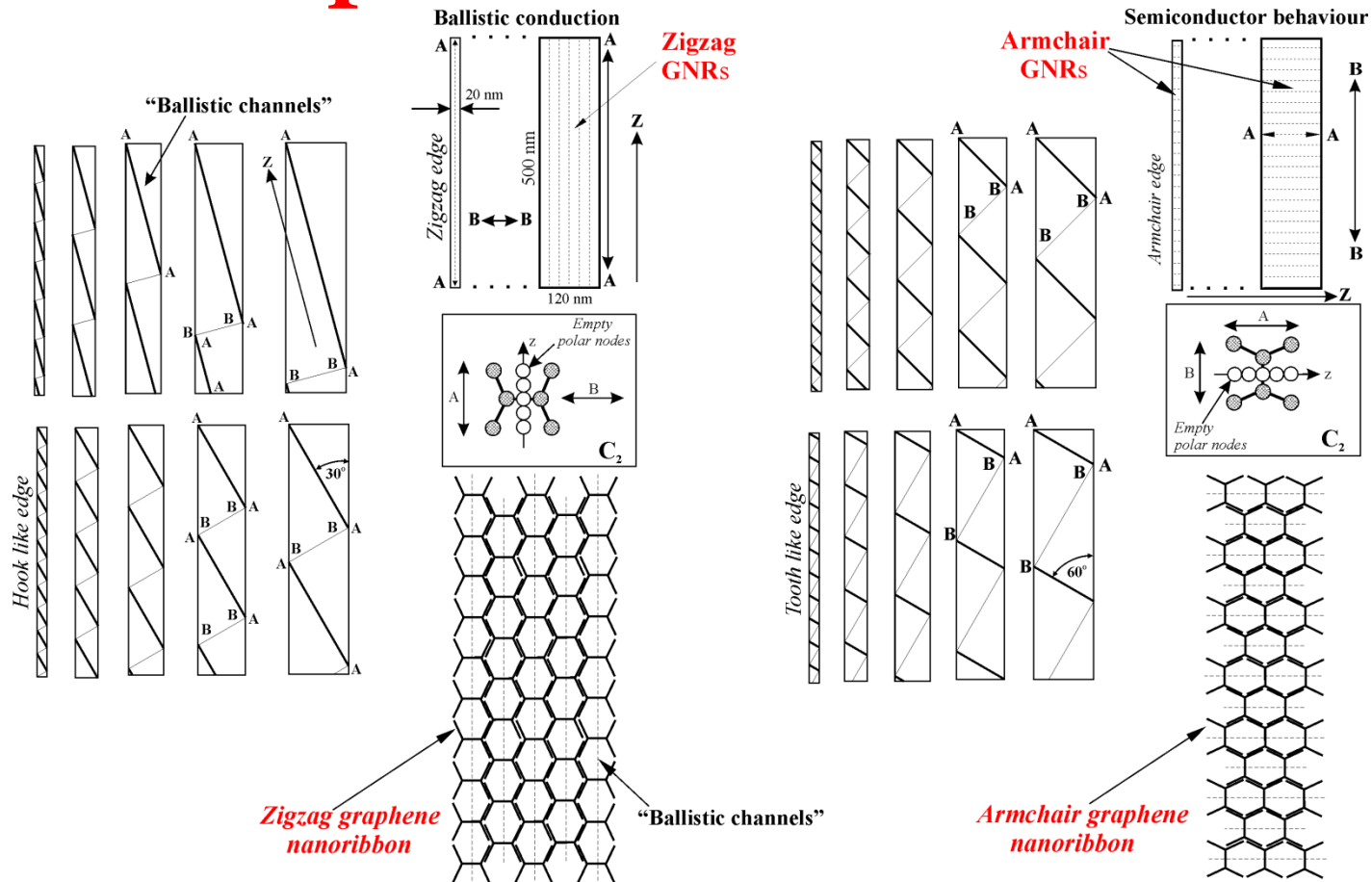
Topological Defects in Graphene
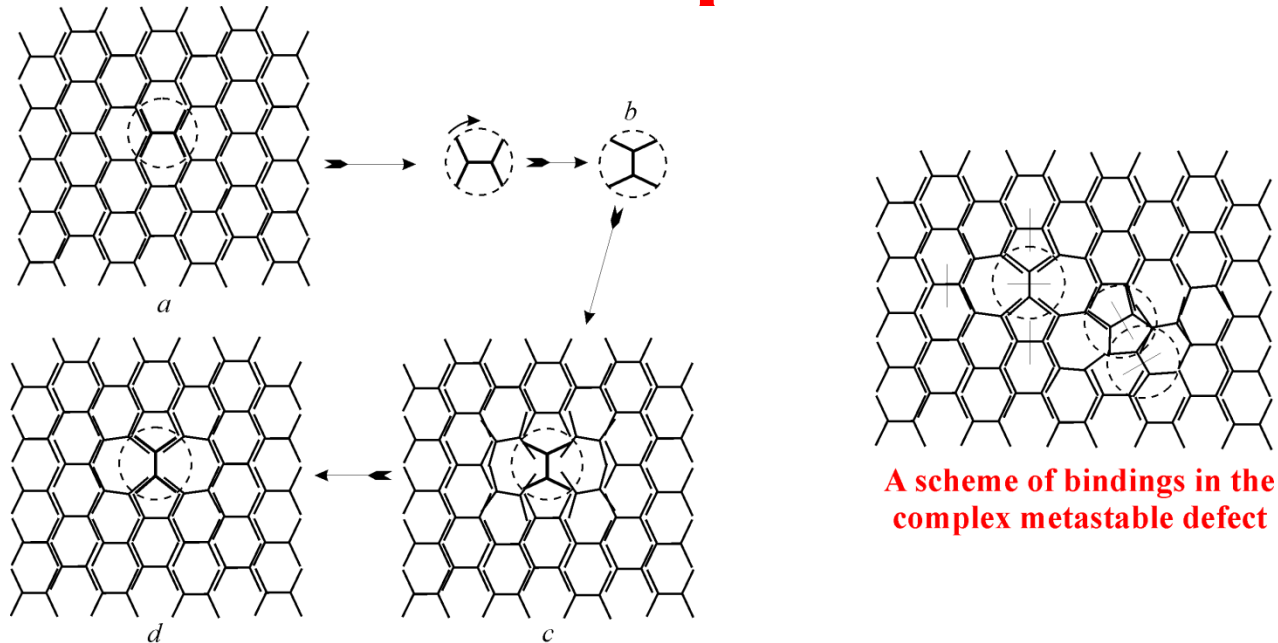
The formation of the pentagon-heptagon (SW) defects

A scheme of bindings in the complex metastable defect

The **pentagon-heptagon** (5-7) (SW) **topological defect** arises due to appearance when heated the **rotational modes** (additionally to vibrational) that leads to violation in some moment of equilibrium bindings resulting in the formation of short-lived bonds with other nodes of nearest carbon dimers, as indicated in this scheme.

Upon cooling it takes place self-organization (self-assembly): an exited region of the lattice returns in the initial equilibrium state, the defect disappears.

Graphene Nanoribbons

Ballistic conduction

Zigzag GNRs

"Ballistic channels"

20 nm

500 nm

120 nm

Zigzag edge

Hook like edge

30°

Empty polar nodes

C_2

Zigzag graphene nanoribbon

"Ballistic channels"

Semiconductor behaviour

Armchair GNRs

Armchair edge

Tooth like edge

60°

Empty polar nodes

C_2

*Armchair graphene nanoribbon*

A **shape** of edges of graphene nanoribbons, different width and length, **depends on orientation of the crystallographic z axis** with respect to the edges.

And the **definite orientation** of the z axis, but not a shape of the edges, **influences on properties** of nanoribbons, for example, on electrical resistance, because the **chains of empty polar nodes,** which are responsible for the **"ballistic" motion of charge carriers**, are directed parallel to this axis (A-A, in the figures).

We should not confuse cause and effect.

The WM concept about the **shell-nodal** structure
of the "atoms" was undergone to direct experimental verification by
detecting the effects caused by the structure

A measurement scheme (*a*)
and SEM image (*b*) of graphene round sheets when tested (2010):
Yes or No anisotropy of conductivity?
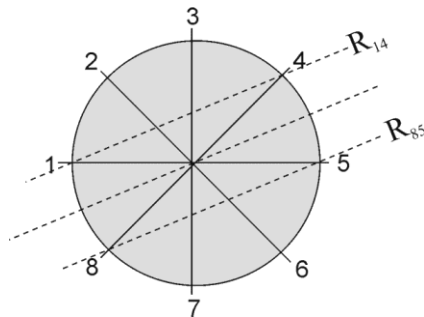
A pair of the identical conductive sections

a)
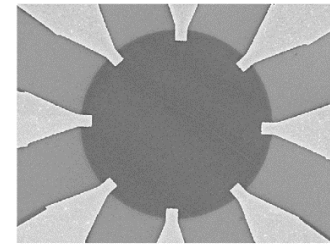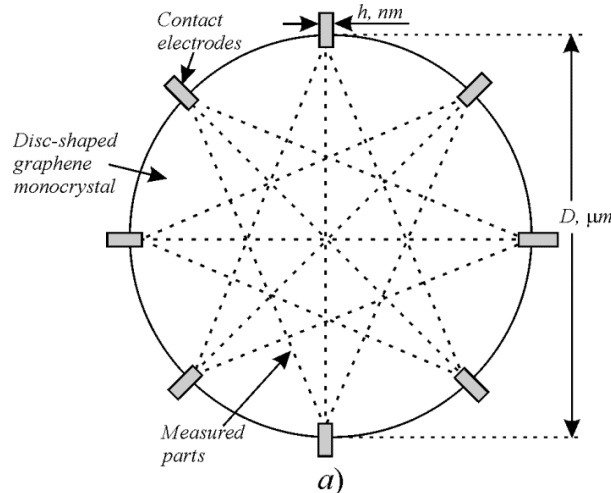
b)

Both resistances between the **parallel pairs of contacts** (e.g., such as R_{14} and R_{85}), embracing identical conductive areas (i.e., having the same geometrical configuration), **must be equal** in value (within the error). This allows providing an **instant control of quality of electric contacts** to disc-shaped graphene plates directly during measuring the resistances.

Therefore, the given **scheme can be used** to test the effectiveness of various technological methods developing for creating improved electric contacts with graphene.

The angular dependence
of electrical resistance R = f(φ)

in a plane of a single graphene sheet of a round form
(D=10 μm, h=580 nm, T=4.2 K, I=1 nA)
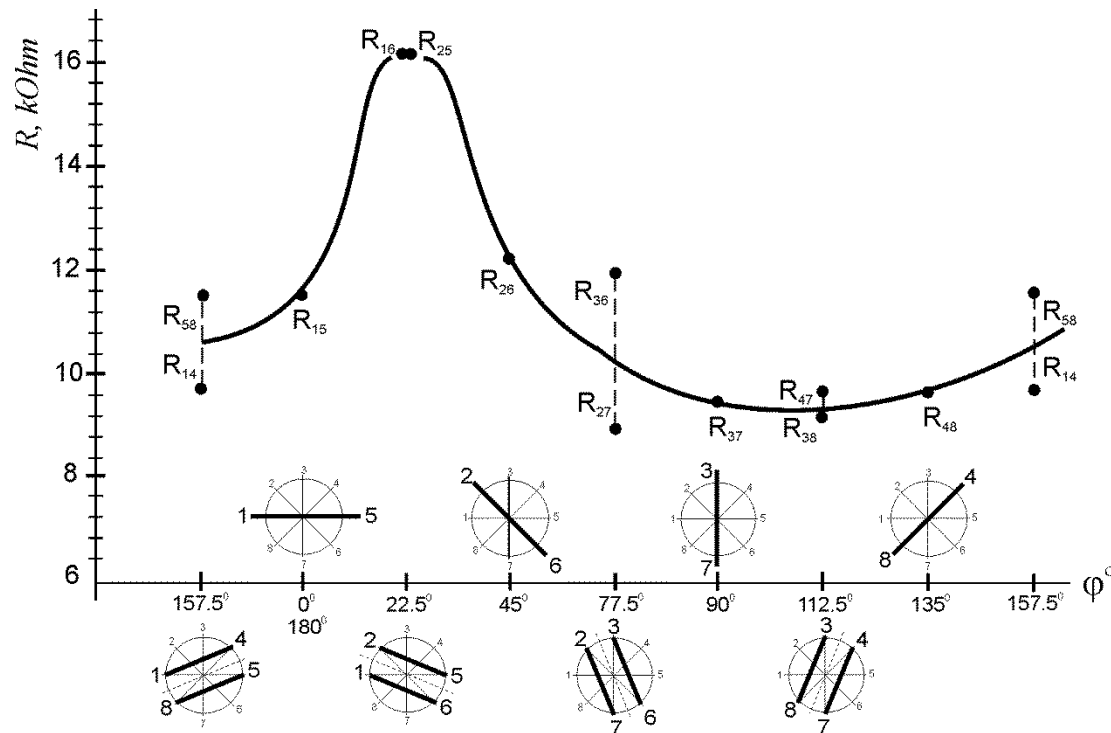
**An obtained dependence is characteristic for anisotropic
materials having the two-fold symmetry**

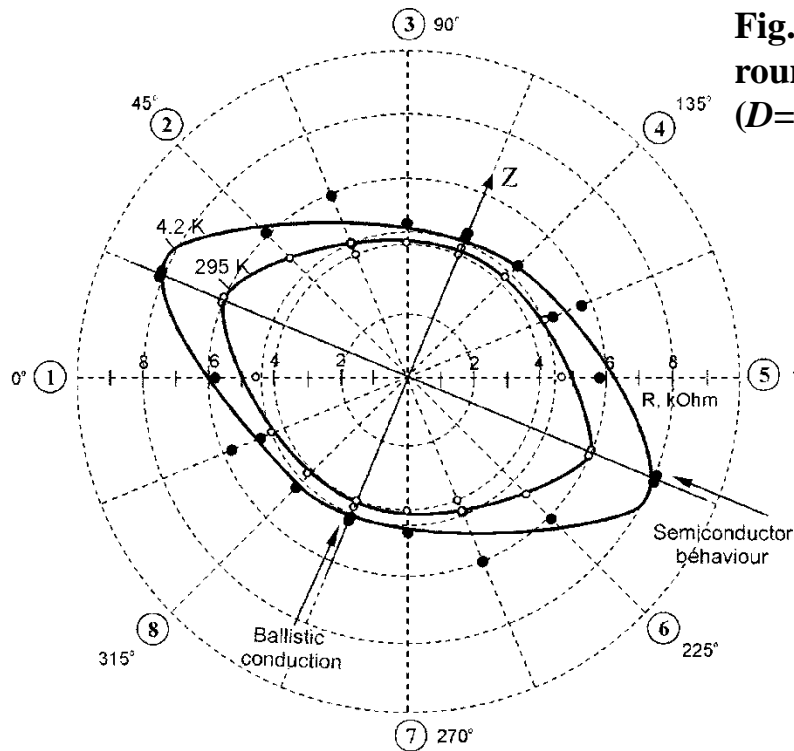# Anisotropic behavior of electrical conductivity in graphene

Fig. A polar diagram of resistance in a plane of a round sheet of graphene in a one-atom thickness: (D=10 μm, h=580 nm, T=4.2 and 295 K)

The **temperature dependence** of graphene conductivity along one of the directions in a plane shows that graphene in this direction **behaves as a semiconductor**.

In the perpendicular direction, along the "ballistic channels" (the z-axis), resistance in graphene practically does not depend on temperature; graphene **behaves as a metal**.

Comparison with a metal refers only to absence of the temperature dependence because the mechanisms of conductivity in a metal and in graphene differ in principle.

Anisotropy of a hexagonal lattice of graphene, predicted theoretically (2009) and confirmed directly experimentally (first in 2010), is the next in a series of the discoveries of the WM, following from the shell-nodal structure of the "atoms" and proving, thereby, reality of the latter (along with the discovery of the nature of all possible "atomic" isotopes)

Anisotropy of unstrained graphene is also well confirmed by optical methods

Obviously, in a case of two-dimensional crystals having a two-fold axis of symmetry, optical parameters of a reflected beam have to be repeated with a period of 180^0 in a plane perpendicular to such an axis.

Therefore, there are no problems of principle to be sure, using optical methods, **whether graphene is isotropic or anisotropic**.

Information about such experiments began to appear in the literature after our statement in February 2009 about the discovery. Here are **two examples**.

- Studies performed by polarized **Raman spectroscopy** (in **2012**) confirmed this feature of unstrained graphene. A prominent sinusoidal intensity modulation with a period of 180^0 is shown below.

- Anisotropy in unstrained pristine graphene (in absence of any external affects) with a periodicity of 180^0 was also confirmed in studies by the **Microscopic Reflection Difference Spectroscopy** in the visible-frequency range (**2014 - 2015**, Beijing Key Laboratory).

Anisotropy in exfoliated graphene sheets

studied by polarized Raman spectroscopy in absence of any external influences (unstrained from outside)*

## A prominent sinusoidal intensity modulation with a period of 180°

The estimated peak positions: 2.647 and 2.660 (a), 2.647 and 2.660 cm^{-1} (b), respectively, for the 2D$^+$ and 2D$^-$ sub-bands.
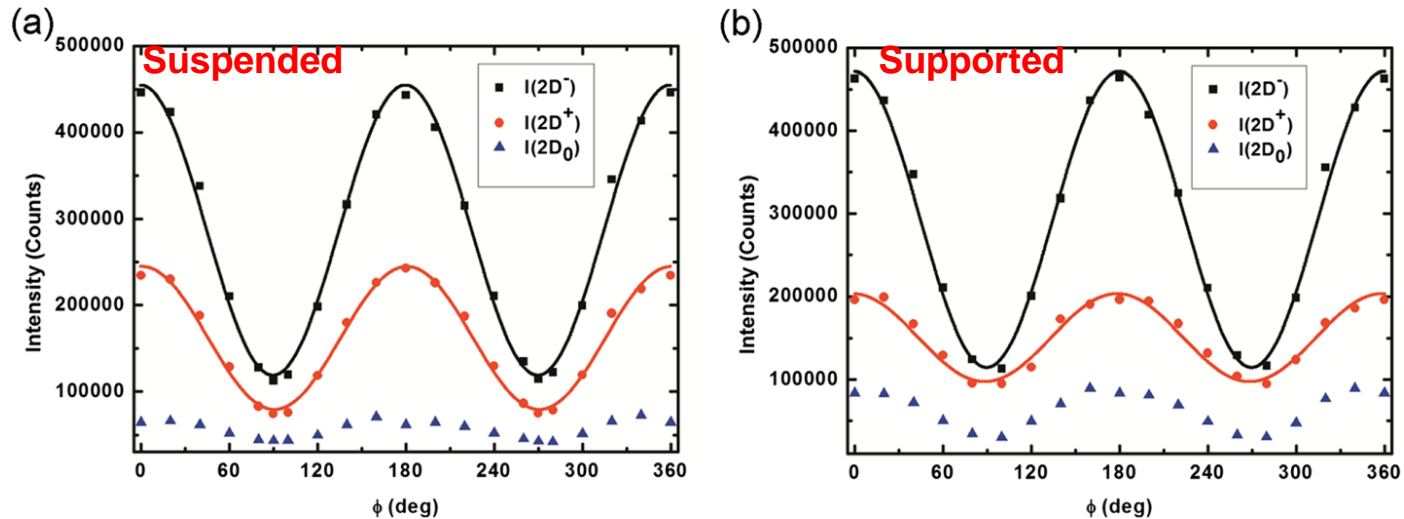
"**Figure 4.** Analysis of intensity. **(a)** Suspended and **(b)** supported graphene. The plots of I(2D$^+$), I(2D$^-$), and I(2D$_0$) as functions of Φ. The symbol 'I' denotes the intensity of the corresponding sub-peak obtained by fitting the related Raman spectrum with a triple-Lorentzian function. The obtained intensities are shown by the dots, which are fitted by the form of Acos^2($\Phi - \Phi_0$) for I(2D$^+$) and I(2D$^-$), and of a constant of A, where A and Φ_0 are fitting parameters. The black and red lines display the fitting results"*.

*[Huang et al, "*Observation of strain effect on the suspended graphene by polarized Raman spectroscopy*", **Nanoscale Research Letters 2012**, 7:533]

By now we have the grounds to argue that **Raman spectra** (presented in different papers, devoted to the influence of strains) reflect, in varying degrees, the natural anisotropy inherent in unstrained graphene. For example, strains, caused by **bending of the hexagonal lattice of graphene** (as in the paper of 29.05.2009* analyzed below), could distort slightly Raman spectra, but not violating, wherein, their main feature.
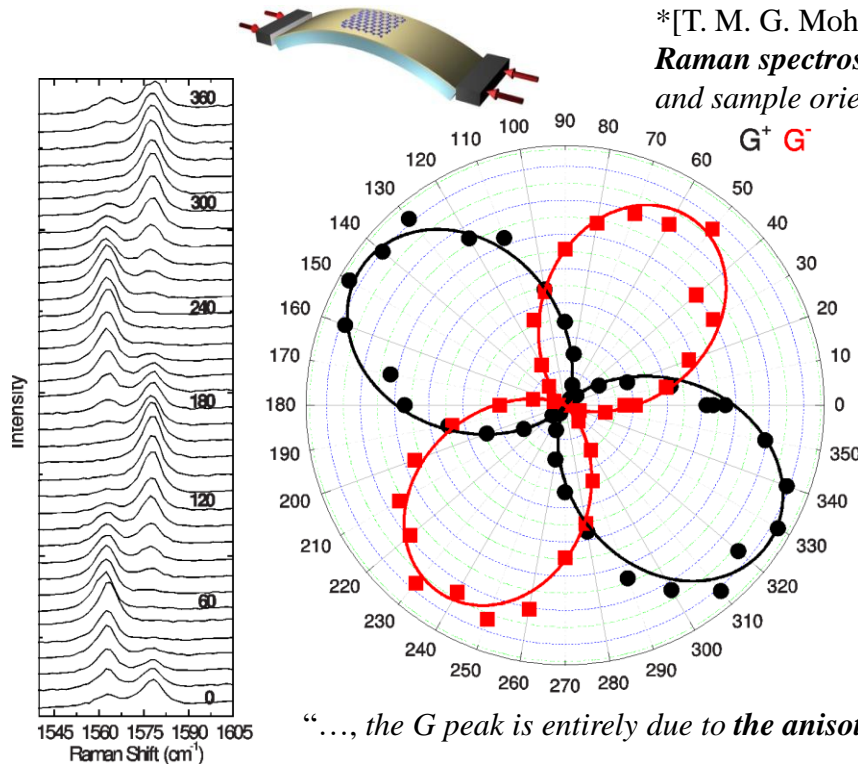
*[T. M. G. Mohiuddin at al, "*Uniaxial strain in graphene by Raman spectroscopy*: G peak splitting, Grüneisen parameters, and sample orientation*", Phys. Rev. B 79, 205433 (29.05.2009)]

FIG. 6. (Color online) (Left) Raman spectra and (right) polar plot of the fitted G^+ and G^- peaks as a function of the angle between the incident light polarization and the strain axis θ_{in} measured with an analyzer selecting scattered polarization along the strain axis $\theta_{out}=0$. The polar data are fitted to $I_{G^-} \propto \sin^2(\theta_{in}+34°)$ and $I_{G^+} \propto \cos^2(\theta_{in}+34°)$, see text.

The extent of strain not indicated here. Why?

"…, the G peak is entirely due to **the anisotropic terms** in the electronic spectrum"

"…, in order to contribute to the G peak, electrons (interacting with phonons, G. Shp.) *must "feel" the* **crystallographic directions**" (page 205433-7)

"*…the inferred strains disagreed by a factor of 5 or more for similar Raman shifts*[20,22-24]" "*…no significance difference was seen between the cases of uniaxial and biaxial strain,*[20,23,24] *in contrast with theory*" (page 205433-1). *Etc*.

Comments to the article*

According to the article*

Strain axis, $\Theta_{out}=0$
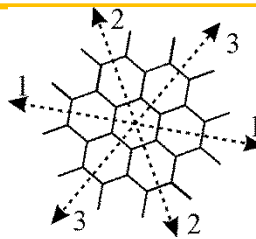
11.3^0

34^0

x

G^+

G^-

C C C C C C

Polar diagram (experiment)
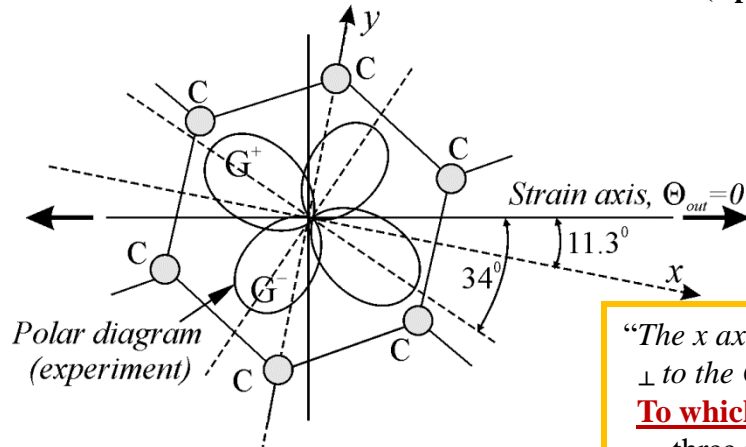
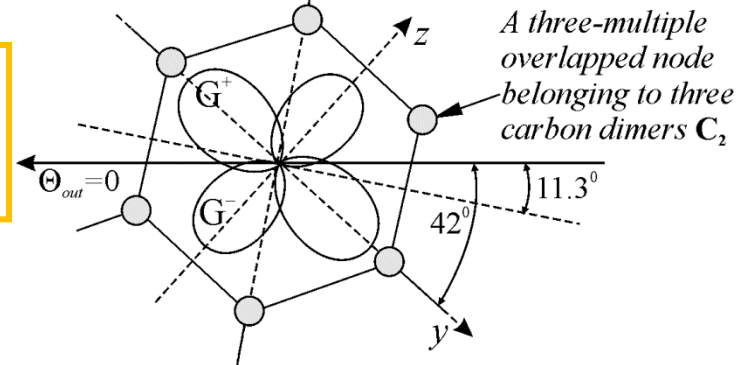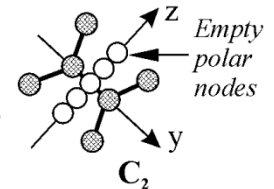Graphene is considered as having **6-fold** rotational symmetry.

Because orientation of the *x* axis is **ambiguous**, the conclusion, "*We thus get the orientation of the graphene crystal with respect to the known strain axis*" (page 205433-6), is **incorrect**.

"*The x axis is chosen* $\perp$ *to the C-C bond*". **To which C-C** of the three identical**?**

2 3
1
1
3 2

Nothing is said about the polar diagram for unstrained graphene. **Why?** Hence, the conclusion about influence of strains on Raman spectra of graphene **can not be considered as correct**.

An expected result for unstrained graphene, in accordance with solutions of the wave equation

z

Empty polar nodes

y

C₂

A three-multiple overlapped node belonging to three carbon dimers **C₂**

$\Theta_{out}=0$

G^+

G^-

z

11.3^0

42^0

y

Graphene has **2-fold** rotational symmetry

Fig. Supposed polar plot of G^+ and G^- peaks as a function of the angle between the incident light polarization and the random crystallographic direction in graphene, as in the paper in question (11.3^0), if it will be measured with an analyzer selecting scattered polarization along this direction, $\Theta_{out} = 0$.

Comparison of two physics models:
conventional and new (SM and WM)

[Phys. Rev. B 79, 205433 (29.05.2009)]

Two different atomic models
(nuclear and shell-nodal, molecule-like)
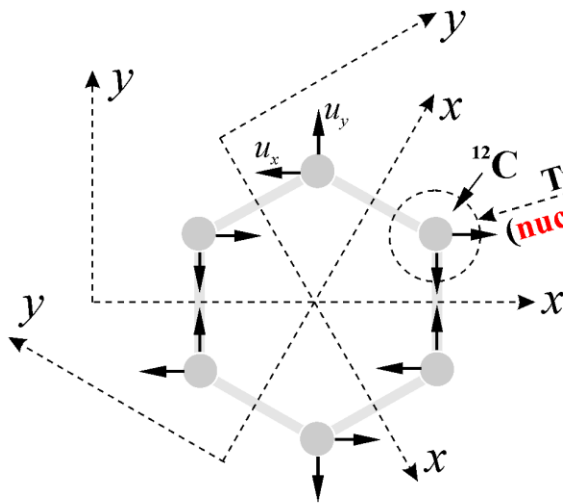
One atom ^{12}C forms each node of the lattice (conventional view)

Small arows indicate
"phonon displacements in the (x,y) basis"
*"The x axis is chosen **perpendicular to** the C-C bond"*
(page 205433-6)
To which of 3 pairs of the identical C-C bonds?

5 empty **polar** nodes invisible by electron microscopy

2 coupled nucleons in each of the 6 **polar-azimuthal** nodes
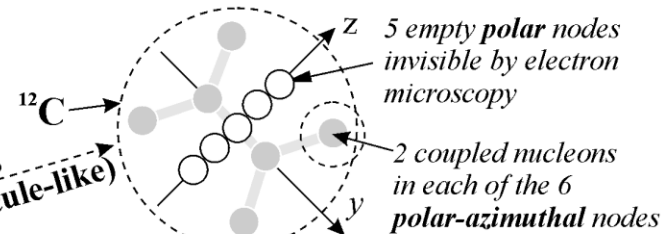
Carbon elementary nucleon molecule ("atom") ^{12}C
(according to the WM)

Crystallographic axis of anisotropy
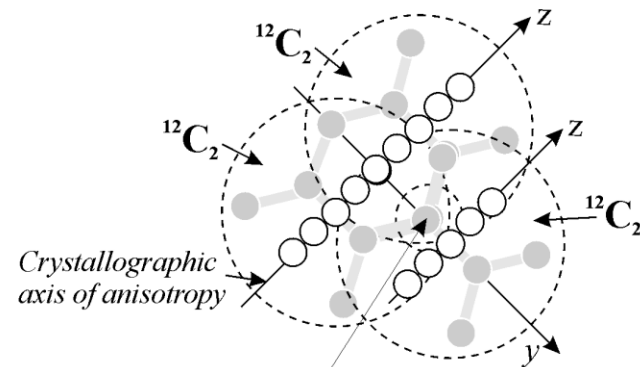
Three nodes, belonging to three carbon dimers ^{12}C$_2$, form, being overlapped, each node of the lattice
(according to the WM)

Thus, independent experiments, carried out by various methods in different laboratories, confirmed our prediction that the **two-fold symmetry is a feature inherent to the hexagonal lattice of graphene.**

Recall that this feature is an **effect of the shell-nodal structure of the carbon "atom" (which is the elementary nucleon molecule)** and specifically ordered bindings of these "atoms" in the hexagonal lattice.

Additional confirmations, as we believe, will be obtained in the ongoing experiments studying a phenomenon of the **Second Harmonic Generation** (SHG), and from other relevant works.

Practical Significance
of the Obtained Results

Predicted and confirmed experimentally, anisotropy of graphene should be taken into account in the electronics industry of the future, which will be based on use of graphene.

The strictly definite orientation of the crystallographic axis of all anisotropic monocrystals on substrates is a mandatory self-evident initial technological stage, which provides electronic devices, produced on such crystals, be identical in parameters.

[G. Shpenkov, ***Method for manufacturing nano electronic devices made from 2D carbon crystals like graphene and devices obtained with this method***", file EP2401764, priority date 29.02.2009; https://register.epo.org/application?number=EP10707863

Particular Conclusion

- **1. Graphene has <u>two-fold</u> rotational symmetry and is an <u>anisotropic</u> crystal.**

- **2. <u>Invisible polar nodes</u>, being bound each other, take the form of parallel <u>hollow channels</u> favourable for the "ballistic" motion of electrons.**

Hence, it becomes understandable and explainable now:

Why *"Graphene...is an interesting mix of a semiconductor...and a metal"* [*]

Why *"Electrons in graphene … have very long mean free paths"* [*].

*[A.H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov and A. K. Geim, ***The electronic properties of graphene***, Rev. Mod. Phys. **81**, 2009]

Why carbon "*Nanotubes can be metallic or semiconducting,…*"

[Tsuneya Ando, ***The electronic properties of graphene and carbon nanotubes***, Review, NPG Asia Materials (2009) 1, 17–21; doi:10.1038/asiamat.2009.1]

Carbon nanotubes, rolled-up form of graphene, have either conductivity, **metallic** or **semiconducting**. The rolling-up is realized mainly along two crystallographic directions: along the major axis of anisotropy and in perpendicular to it direction. They define the thermodynamically favourable minimum-energy states.

General Conclusion

We highlight here

three breakthrough discoveries

(from a series of others made within the WM),

which alter our conventional ideas regarding the structure of matter:

● **1.** "Atoms", being stable wave formations, have the <u>shell-nodal structure</u> and are <u>elementary nucleon molecules.</u> Their nodes, filled with paired hydrogen atoms, are bound to each other by <u>strong interaction</u>.

● **2.** The main role at the formation of molecules and crystals plays a <u>spatial arrangement of the nodes</u> and <u>internodal strong bonds</u> in the "atoms". Electrons play the secondary role: <u>they define only the strength of chemical bonds</u>.

Chemical "covalent" bonds are realized directly along strong internodal bonds each of the joined "atoms" or their dimers.

● **3.** <u>All "atomic" isotopes</u> (their structure and relative mass) are defined by the extent of filling all potential and potential-kinetic nodes of the "atoms" with hydrogen atoms.

Judging by the results, the WM has to be considered as an alternative to the Standard Model

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Summary

The direct fundamental evidences,
obtained by the author within the Wave Model,

testifying to the reality the nuclear-free shell-nodal (molecule-like) structure of the "atoms"

● **Proven experimentally** (and confirmed independently in different laboratories) **anisotropy of unstrained graphene** caused by the specific shell-nodal structure of carbon elementary nucleon molecules (carbon "atoms").

● **Derived** the structure and relative masses of a full set of all natural and artificial "atomic" isotopes. They are grouped in the "**Table of the "Atomic" Isotopes**".

● **Derived** the binding energy of the "atoms" (deuterium, tritium, helium $_2^4 He$, and carbon $_6^{12} C$) and internodal bindings in molecules by the **Universal Law of the Central Exchange**, $F_e = \omega_e^2 \dfrac{m_1 m_2}{4\pi\varepsilon_0 r^2}$, discovered in the WM, where $\varepsilon_0 = 1\, g \cdot cm^{-3}$ is the absolute unit density, $\omega_e = 1.869162559 \times 10^{18}\, s^{-1}$ is the *fundamental frequency* of atomic and subatomic levels; m_1 and m_2 are associated masses of exchange defined by Eq. $m = \dfrac{4\pi r^3 \varepsilon_0 \varepsilon_r}{1 + k_e^2 r^2}$, and $k_e = \omega_e / c$ is the wave number.

● **Revealed** that the strictly *certain distances between nucleon* nodes in substance are defined by the *fundamental wave radius* $\lambdabar_e = c / \omega_e = 1.60...\times 10^{-8}\, cm$. E.g., ***lattice parameters*** are equal in average to $2\lambdabar_e \approx 3.2 \times 10^{-8}\, cm$. Distances r between nodes in the "atoms" (nucleon molecules) are defined by the product $z_{m,n}\lambdabar_e = r$, where $z_{m,n}$ are roots of Bessel functions.

● **Revealed** that *characteristic angles of facets* in crystals of natural minerals are determined by the same particular solutions as spatial angles of the nodes in "atoms". This confirms the *wave nature of natural minerals*, and, generally, of all substances.

● **Explained** the **scattering of particles and waves on nuclear-free "atoms"** (i.e., on nucleon nodes of the bound elementary molecules in substance)**,** completely agreed with the experiment. It was made naturally and logically noncontradictory, as against questioned contradictory Rutherford' explanation of the scattering on hypothetical tiny hyperdense atomic nuclei [4].

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