

BOOK REVIEW

BOOK REVIEW: PERIODIC NANOSTRUCTURES, BY DIUDEA M.V. AND NAGY C.L., ISBN 978-1-4020-6019-9, SPRINGER, JUNE 2007

Lorentz Jäntschi

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INTRODUCTION

The book *Periodic Nanostructures* is part of Springer series *Developments in Fullerene Science*, being 7-th book published in this series. Authors of this book are both from Cluj, Romania, and affiliated to "Babeş-Bolyai" University of Cluj-Napoca.

First author of the book, Mircea Vasile DIUDEA was the Ph.D. advisor of the author during his Ph.D. preparation (1997-2000).

Before starting to present this book, let do a retrospective of advances to modern biochemistry (see Table 1).

Table 1. Advances to modern biochemistry till 1990

Biology	Years	Chemistry and Physics
Cell nuclei; Cell theory	1830-1849	Urea synthesis
	1850-1869	Chemistry as tool for biological characterization
Genetic discovering of DNA	1870-1889	
Drosophila genetics	1890-1909	Fermentation discovery; Urease crystallization
Electronic microscopy	1910-1929	Glycolysis characterization
DNA functions	1930-1949	Citric acid cycle characterization
X-ray analysis for proteins from restriction enzymes	1950-1969	DNA double chain; Genetic code
Catalytic RNA; Genetic therapy	1970-1989	Recombinant DNA; Polymerase chain reaction

Coming to the present, a remarkable advance was realized by the use of computers. I will mention just three examples.

The paper *Computer Assisted Rational Design of Immunosuppressive Compounds* (Authors Grassy G., Calas B., Yasri A., Lahana R., Woo J., Iyer S., Kaczorek M., Floc'h R., Buelow R., Nature Biotechnology, 1998, 16, p. 748-752 reports on a search for peptides possessing immunosuppressive activity. They used 27 structure descriptors. From a combinatorial library of about 280000 virtual compounds, they selected 26 peptides for which high activity was predicted. Five of them were actually synthesized and tested experimentally. The most potent of these shown an immunosuppressive activity approximately 100 times higher than the lead compound.

Sequencing of human DNA is another challenge, which cannot be made without computations. Note that more than three billion nucleotides are in a haploid human genome. In 2001, the International Human Genome Sequencing Consortium reported a draft sequence of the euchromatic portion of the human genome [The Sequence of the Human Genome, Venter C. J. & all, Science, 2001, 291(5507), p. 1304 - 1351]. Human genome sequence was considered pragmatically 'complete' at 92% in 2005 in publications by an international public HGP and somewhat independently by a private company Celera Genomics. In 2006, another milestone was passed on the way to completion of the project, when the sequence of the last chromosome was published in the journal Nature [Erratum: The DNA sequence and biological annotation of human chromosome 1 (Nature (2006) 441 (315-321)), Gregory S.G. & all, Nature, 2006, 443(7114), p. 1013]. At the end, it must be mentioned that the largest database containing genome sequences are at the National Health Institute [Genome sequencing project at International Human Genome Sequencing Consortium]. Let's cite from here the lineage: Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini; Catarrhini; Hominidae; Homo; Homo sapiens.

Not such DNA complex structures are nanostructures, but also is a challenge. Eiji Osawa from Toyohashi University of Technology predicted the existence of the C₆₀ in 1970, when he noticed that the structure of a corannulene molecule was a subset of a soccer ball, and made the hypothesis that the full ball could exist too. Later, in molecular beam experiments, discrete peaks were observed corresponding to molecules with the exact mass of sixty or seventy or more carbon atoms. In 1985, Harold Kroto (then of the University of Sussex, now of Florida State University), James R. Heath, Sean O'Brien, Robert Curl and Richard Smalley, from Rice University, discovered C₆₀, and shortly after came to discover the fullerenes. The next advance was made doing computations on fullerenes structure. Aggregated diamond nanorods, or ADNRs, are an allotrope of carbon predicted to be the least

compressible material known to humankind, as measured by its isothermal bulk modulus are one of the latest challenges [What does 'harder than diamond' mean?, Brazhkin V., Dubrovinskaia N., Nicol M., Novikov N., Riedel R., Solozhenko V., Zhao Y., *Nature materials*, 2004, 3(9), p. 576-577]. Recently, predictions again were proved by the experiment. A process to produce the aggregated diamond nanorods was discovered by physicists in Germany, led by Natalia Dubrovinskaia, at the University of Bayreuth in 2005 [Nanocrystalline diamond synthesized from C_{60} , Dubrovinskaia N., Dubrovinsky L., Langenhorst F., Jacobsen S., Liebske C., *Diamond and Related Materials*, 2005, 14(1), p. 16-22].

Novel carbon allotropes, such as spherical fullerenes and nanotubes, have been added, in the last three decades, to the traditionally recognized diamond and graphite. Although fullerene C_{60} has been speculated about for a long time. A fullerene is, according to a classical definition, an all-carbon molecule consisting entirely of pentagons (exactly 12) and hexagons ($n/2-10$). Non-classical fullerene extensions to include rings of other sizes have been considered. Fullerenes are commonly synthesized by arc-discharge or laser ablation methods. Spherical fullerenes became nowadays parts of real chemistry: they can be functionalized or inserted in supramolecular assemblies. From supramolecules applications, let cites [Organophosphorus supramolecular chemistry part 1. Receptors for organophosphorus compounds, Berlicki L., Rudzińska E., Młnarz P., Kafarski P., *Current Organic Chemistry*, 10(18), 2006, p. 2285-2306]: "In this review a state-of-the-art research showing current progress in design and application of host molecules able to recognize and bind specifically phosphate, phosphonate or phosphinate fragments is described. These molecules are usually designed as chemical models of chosen enzymes or for various analytical purposes (as components of sensors, extractants, chiral discriminators, membrane carriers ect.)".

Book content

The book has seven chapters: Periodic fullerenes by coalescence reactions, Polyhex tori, New classes of toroidal structures, Counting polynomials of nanostructures, Operations on maps, Tromaticity of nanostructures, and Triply periodic nanostructures.

Periodic fullerenes by coalescence reactions chapter contains Fullerene fusion via stone-wales transformation, Results and discussion, Closed nanotubes viewed as coalescence products, Armchair and zigzag closed nanotubes, and Energetics of capped nanotubes.

Polyhex tori chapter contains Construction of polyhex tori from square tiled tori, Topology of polyhex tori, Strain energy calculation, p-Electronic

structure of polyhex tori, Identical polyhex toroidal graphs, and Resonance energy in polyhex tori.

New classes of toroidal structures chapter contains Distinct walled tori, Conetori, and Diameter doubling of SWNT.

Counting polynomials of nanostructures chapter contains Graph theory background, Counting polynomials, Layer/shell matrices and polynomial coefficients, Basic Cluj polynomials, Properties of the Cluj polynomials, Omega-type polynomials, Hosoya polynomial in toroidal nanostructures, Omega polynomial in tubular nanostructures, and QSPR studies by omega-derived descriptors.

Operations on maps chapter contains Simple operations on maps, Composite operations on maps, Generalized operations, and Isomerization routes on tubular nanostructures.

Aromaticity of nanostructures chapter contains Aromaticity of nanostructures, Corannulenic cages, Corazulenic cages, and Retro Endo-Kroto reaction.

Last chapter, Triply periodic nanostructures contains Background on surface curvature, Carbon lattices embedded in TPMSs, Nanotube junctions, and Pedriodic schwarzites.

About the book

Periodic Nanostructures book cumulates the knowledge about the periodicity in various nanostructures. The text covers the coalescence reactions, and shows that the nanoworld is continuous, giving rise to zero- (fullerenes), one- (tubules), two-(graphite) and three-(diamond, spongy carbon) dimensional carbon allotropes.

Exploring of foam-like carbon structures, related to 'schwarzites', which represent infinite periodic minimal surfaces of negative curvature shows that these structures contain polygons (with dimensions larger than hexagons w.r.t. to graphite) that induce this negative curvature. The units of these structures appear as nanotube junctions (produced via an electron beam) that have wide potential molecular electronics applications.

The text provides literature and data on nanostructure periodicity and own results on nanostructure building and energy calculations as well as topological characterization by means of counting polynomials of periodic nanostructures. The aromaticity of various coverings of graphitic structures is also discussed using this approach.

Self-assembled supramolecular structures (of various tessellation) and diamond architectures are treated. The authors propose that the periodicity of close repeat units of such structures is most evident not only in these formations but also present in all of the carbon allotropes. It is shown that depending on the lattice tessellation, heteroatom type, and/or doping, metal nanostructures (nanotubes in particular) can display both metallic and semiconductor characteristics. Therefore, their properties can be controlled via chemical design. The

authors therefore suggest that nanostructures have heralded a new generation of nanoscale biological, chemical, and physical devices.

About Prof. Dr. Mircea V. DIUDEA

Professor Dr. Mircea V. DIUDEA is from Organic Chemistry Department of Faculty of Chemistry and Chemical Engineering from “Babeş-Bolyai” University of Cluj-Napoca. He is founder of Molecular Topology Group, at 20th anniversary in 2006 [Mircea V. DIUDEA (organizer), TOPMOL2006 - 20 Years Anniversary of Molecular Topology at Cluj, Babes-Bolyai University, CEEEx M3 PR-D11-PT00-41, Cluj-Napoca, Romania, September 25-30, 2006], and also is founder of the European Society of Mathematical Chemistry (in 2007).

Prof. M. V. Diudea published numerous books in prestigious publishing houses, promoting in same time his Ph.D. Students. M. V. Diudea and G. Katona, 1999 - Molecular Topology of Dendrimers (book chapter), in Newkome, G.A. (Ed.), Advances in Dendritic Macromolecules (series), 4, pages 135-201, Elsevier, Stamford, Connecticut, USA, ISBN 978 -0-7623 – 0347 - 2 (G. Katona being his Ph.D. Student); Diudea M.V., Gutman I., Jäntschi L., 2001 - Molecular Topology, 332 pages, Nova Science, Huntington, New York, USA, ISBN 978-1-56072-957-0 (L. Jäntschi being his Ph.D. Student).

Prof. M. V. Diudea edited two books: Diudea M. V. (Ed.), 2001 - QSPR/QSAR Studies by Molecular Descriptors, 438 pages, Nova Science, Huntington, New York, ISBN 978-1-56072-859-0 (where other of his Ph.D. Student was invited to contribute, O. Minailiuc) and Diudea M. V. (Ed.), 2005 - Nanostructures: Novel Architectures, 420 pages, Nova Science, Huntington, New York, USA, ISBN 978-1-59454-499-9 (where other of his Ph.D. Students were invited to contribute: C. Nagy, M. Ştefu, and D. Butyka).

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AUTHOR'S ADDRESS

JÄNTSCHI LORENTZ - Technical University of Cluj-Napoca, Romania, 103-105 Muncii Bvd., 400641 Cluj-Napoca, Cluj, Romania,
<http://lori.academicdirect.org>, email:
lori@academicdirect.org