

Autobiography of Mircea V. Diudea



Professor Mircea V. Diudea is born in 1950, November, 11, in Silivas, a village of Transylvania, Romania, in a family of primary school teachers. He followed the high school “Nicolae Balcescu”, Cluj and next the Faculty of Chemistry, University of Cluj (1969-1974). The PhD thesis, entitled “Phenothiazines and related structures” (performed in organic synthesis, under the guiding of two bright Chemists, Professors Valer Farcasan and Cornel Bodea) was defended in 1979, at the Institute of Chemistry, Cluj. He worked six years (1974-1980) as a chemist at “Terapia” Drug Factory, Cluj and the next seven years (1980-1987) as researcher, at Chemical-Pharmaceutical Research Institute, Cluj. From 1987 was admitted at the Faculty of Chemistry and Chemical Engineering, of “Babes-Bolyai” University, Cluj, as assistant professor (1987-1990), next as associate professor, (1990-1996) and from 1996 as full professor, at the Department of Organic Chemistry. His main courses in Chemistry: Organic Chemistry and Biologically Active Compounds.

In 1986 he established the TOPO GROUP CLUJ, and in 2007 founded the European Society of Mathematical Chemistry ESMC, of which first president is. These data include a period of 21 years when a new interdisciplinary science called Molecular Topology has been developed under his guidance and resulted in publication of more than 250 scientific articles (Hirsch index 23 (ISI) or 26 (Scopus), with more than 1200 citations in ISI journals) and 14 authored or edited books, in three directions:

1. **Molecular Topology** (basic theory, with the main results including matrices (Cluj, shell, combinatorial, matriceal operators), topological indices (Cluj, Cluj-Ilmenau, Cluj-Tehran, super-index Cluj-Niš, index of centrality, centric connectivity index, etc.) and

algorithms (for inter and intra-molecular ordering, topological symmetry/equivalence classes of subgraphs, for enumerating the Kekulé valence structures).

2. **QSAR/QSPR** (correlating studies, with contributions in: data reduction procedures, clustering procedures based on 2D and 3D similarity, optimal regression procedures, modeling various physico-chemical properties and biological activities, algorithms for 2D and 3D similarity and drug design).

3. **Nanoscience** (basic theory, with contributions in: Design of nanostructures by operations on maps and nets, the Romanian “Capra” being the first pro-chiral basic operation, rules of stability of fullerenes, a modified Euler theorem in multi-shell nanostructures, original counting polynomials: Omega, Pi, Theta, Cluj, the new diamond D₅ (hoped to be produced in the NanoLab of Carbon Allotropes, organized under his guidance), a Gallery of molecular art, etc).

The scientific activity in his group is supported by 10 original software programs. As didactical activity, Mircea Diudea delivered courses of Molecular Topology, QSAR/QSPR and Fullerenes and Nanostructures, basically at Master and PhD levels (with 12 PhD theses defended so far).

Professor Mircea Diudea is member of International Academy of Mathematical Chemistry (2005) and member of Editorial Board of: *Croatica Chemica Acta*, *MATCH*, *Communications in Mathematical and in Computer Chemistry*, *Internet Electronic Journal of Molecular Design*, *Carpathian Journal of Mathematics*, *Iranian Journal of Mathematical Chemistry*, *Acta Universitatis Cibiniensis* and Senior Editor at *International Journal of Chemical Modeling*, NOVA Publishers, New York, USA. Also he is a referee at the following scientific journals:

(1) *Rev. Roum. Chim.*, (2) *Studia Univ. Babes-Bolyai*, (3) *Croat. Chem. Acta*, (4) *J. Chem. Inf. Comput. Sci.*, (5) *Chem. Phys. Lett.*, (6) *Int. Elect. J. Mol. Design*, (7) *New J. Chem.*, (8) *SAR/QSAR Env. Res.*, (9) *Bioorg. Med. Chem. Lett.*, (10) *MATCH Commun. Math. Comput. Chem.* (11) *Fullerenes, Nanotubes Carbon Nanostruct.*, (12) *Molecules*, (13) *J. Am. Chem. Soc.* (14) *Romanian Chemical Quarterly Reviews*, (15) *Ars Combinatorica*, (16) *Arkivoc*, (17) *Utilitas Math*, (18) *Eur. J. Operational Res.*, (19) *Math. Comput. Model.*, (20) *J. Math. Chem.*

In the list of his stages of international collaboration, invited lectures, conferences, the following are included: Zelinsky Institute of Organic Chemistry, Russian Academy, Moscow, Russia, Rudger Bošković Institute, Zagreb, Croatia, Central Chemical Research Institute of Hungarian Academy, Budapest, Hungary, University of Bayreuth, Germany (as a DAAD fellowship), Technical University of Ilmenau, Germany, University of Bielefeld, Germany (as a second DAAD fellowship), University of Kiel, Germany, Forschungszentrum, Institut für Nanotechnology, Karlsruhe, Germany, University of Karlsruhe, Germany, University of Erlangen, Germany, University of Exeter, UK, University of Hiroshima, Japan, University of Sendai, Japan, University of Tsukuba, Japan (five months), Catholic University Leuven, Belgium, University of Gent, Belgium, University of Sheffield, U.K., University of Miskolc, Hungary, National Institute of Chemistry, Ljubljana, Slovenia, University of Valencia, Spain,

University of Milano-Bicocca, Italy, University of Tehran, Iran, Technical University, Isfahan, Iran, University of Warsaw, Poland, Collegium Budapest, Hungary, - University of Kashan, Iran, University of Shiraz, Iran, Tarbiat Modares University, Tehran, Iran, State University, St. Petersburg, Russia, University of Ljubljana, Slovenia).

Professor Diudea met the Iranian leaders in Mathematics and Mathematical Chemistry in Gent, Belgium, 2006. Since then, a fruitful collaboration has been established between Romanian TOPO GROUP CLUJ and Iranian scientists, resulted in 28 scientific articles (see the list attached), participation at Math. Chem. Conferences, both in Romania and Iran. Professor Diudea participated, between 2008-2010, at a joint Project entitled: Counting Polynomials of Nanostructures, project supported by Iranian National Science Foundation (INSF).

Books (authored):

1. M. V. Diudea, S. Todor, F. Igna, *Aquatic Toxicology*. DACIA, Cluj, 1986 (in Romanian). 320p.
2. M. V. Diudea, M. Pitea, M. Butan, *Fenothiazines and structurally related drugs*. DACIA, Cluj, 1992 (in Romanian)., 278p.
3. M.V. Diudea, O. Ivanciuc, *Molecular Topology*, COMPREX, Cluj, 1995 (in Romanian), 320p.
4. M.V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology*, NOVA, New York, 2002. , 329p.
5. M. V. Diudea, M. S. Florescu, and P. V. Khadikar, *Molecular Topology and Its Applications*, EFICON, Bucharest, 2006, 381 pp. (Eficon Press, Bucuresti, ISBN 978-973-87904-0-7)
6. M. V. Diudea, Cs. L. Nagy, *Periodic Nanostructures*, SPRINGER, 2007 (207p).
7. M. V. Diudea, *Nanomolecules and Nanostructures – Polynomials and Indices*, M C M, No. 10, University of Kragujevac, 2010 (472p).

Edited Books (Ed):

- 1.M. V. Diudea, *QSPR/QSAR Studies by Molecular Descriptors*, NOVA, New York, 2001., 438p.
- 2.M. V. Diudea, *Nanostructures, Novel Architecture*, NOVA, New York, 2005, 420pp.

Journal Issues (Guest Ed):

1. M. V. Diudea, O. Ivanciuc, *MATCH Commun. Math. Comput. Chem.*, 2001., **44**, 428p.
2. M. V. Diudea, *Internet Electron. J. Mol. Des.*, 2002, **1** (1-6), 427p.
3. M. V. Diudea, *J. Math. Chem.*, 2009, **45**.
4. M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, 2008, **60**.
5. M. V. Diudea, *Symmetry: Culture and Science*, 2008, **19**.

Book Chapters

1. M. V. Diudea and G. Katona, Molecular Topology of Dendrimers. In: Newkome, G.A. Ed., *Advan. Dendritic Macromol.* 1999, **4**, 135-201.
2. O. M. Minailiuc and M. V. Diudea, TI-MTD Model. Applications in Molecular Design. In: M. V. Diudea, Ed., *QSPR/QSAR Studies by Molecular Descriptors*. NOVA, New York, 2001, pp. 363-388.
3. Cs. L. Nagy, M. V. Diudea, and T. S. Balaban, Coalescence of fullerenes. In: M. V. Diudea, Ed., *Nanostructures-Novel Architecture*, NOVA, New York, 2005, 25-60.
4. M. V. Diudea, Cs. L. Nagy and A. Graovac, Periodic Finite Nanostructures. In: M. V. Diudea, Ed., *Nanostructures-Novel Architecture*, NOVA, New York, 2005, 61-84.
5. M. V. Diudea, Covering Nanostructures, In: M. V. Diudea, Ed., *Nanostructures-Novel Architecture*, NOVA, New York, 2005, 203-242.
6. M. Stefu, D. Butyka, M. V. Diudea, L. Jantschi, and B. Parv, Algorithms for basic operations on maps, In: M. V. Diudea, Ed., *Nanostructures-Novel Architecture*, NOVA, New York, 2005, 243-267.
7. M. Stefu and M. V. Diudea, Distance Counting in Tubes and Tori: Wiener Index and Hosoya polynomial. In: M. V. Diudea, (Ed.), *Nanostructures–Novel Architecture*, Nova, New York, 2005, 127-165.
8. Cs. L. Nagy and M. V. Diudea, Nanoporous carbon structures, In: M. V. Diudea, (Ed.), *Nanostructures–Novel Architecture*, Nova, New York, 2006, 311-334.
9. M. V. Diudea, Covering nanostructures, in: A. Graovac, I. Gutman, and D. Vukicevic, Eds., *Mathematical Methods for Students of Chemistry and Biology*, Proceedings of the MMC 2007, Hum, Zagreb, 2009.
10. M. V. Diudea, Nanostructure design - between science and art, in: M. Putz, Ed., NOVA, 2009.
11. E. Vizitiu and M. V. Diudea, C₆₀ Structural Relatives-An Omega-aided Topological Study, in: A. Graovac, A. Ottorino, Eds. 2010.
12. M. V. Diudea, Counting polynomials in partial cubes, in: I. Gutman, Ed., *New Topological Descriptors*, MCM series, MATCH, 2010.
13. A. Ilić, F. Gholami-Nezhaad, A. Vizitiu and M. V. Diudea, Counting polynomials and indices in Nanocones, in: I. Gutman, Ed., *New Topological Descriptors*, MCM series, MATCH, 2010.
14. M. V. Diudea, M. Petitjean, Symmetry in multi tori, in: M. V. Diudea (Ed), *Simmetry, Culture, Sci.*, 2008, **19** (4), 285-305

Representative articles:

1. M. V. Diudea, Cluj polynomials, *J. Math. Chem.*, 2009, **45**, 295 -308.
2. M. V. Diudea, Omega Polynomial, *Carpath. J. Math.*, 2006, **22**, 43-47.
3. M. V. Diudea, Hosoya polynomial in tori. *MATCH Commun. Math. Comput. Chem.*, 2002, **45**, 109-122.
4. M. V. Diudea, D. Vukicevic, Kekule structure count in corazulenic fullerenes, *J. Nanosci. Nanotechnol.*, 2007, **7**, 1321–1328.

5. Sh. Xu, H. Zhang, M. V. Diudea, Hosoya polynomials of zig-zag open-ended nanotubes, *MATCH Commun. Math. Comput. Chem.*, 2007, **57**(2), 443-456.
6. R. B. King and M. V. Diudea, The chirality of icosahedral fullerenes: a comparison of the tripling (leapfrog), quadrupling (chamfering), and septupling (capra) transformations, *J. Math. Chem.* 2006, **39**(3-4), 597-604.
7. O. Ursu, M. V. Diudea and Sh-i. Nakayama, 3D Molecular similarity: method and algorithms, *J. Comput. Chem. Jpn.*, 2006, **5**, 39-46.
8. M. V. Diudea, Nanoporous carbon allotropes by septupling map operations, *J. Chem. Inf. Model.*, 2005, **45**, 1002-1009.
9. M. V. Diudea, Corannulene and corazulene tiling of nanostructures, *Phys. Chem., Chem. Phys.*, 2005, **7**, 3626-3633.
10. M. V. Diudea, Covering Forms in Nanostructures, *Forma (Tokyo)*, 2004, **19** (3), 131-163.
11. M. V. Diudea, Stability of tubulenes, *Phys. Chem., Chem. Phys.*, 2004, **6**, 332-339.
12. M. V. Diudea and Cs. L. Nagy, Euler Formula in Multi-Shell Polyhedra, *MATCH Commun. Math. Comput. Chem.*, 2008, **60**, 835-844.
13. M. V. Diudea, Phenylene and naphthalene tori. *Fullerenes, Nanotubes Carbon Nanostruct.*, 2002, **10**, 273-292.
14. M. V. Diudea, M. Ștefu, P. E. John, and A. Graovac, Generalized operations on maps, *Croat. Chem. Acta*, 2006, **79**, 355-362.
15. P. E. John, A. E. Vizitiu, S. Cigher and M. V. Diudea, CI Index in Tubular Nanostructures, *MATCH Commun. Math. Comput. Chem.*, 2007, **57**(2), 479-484.
16. M. Lillington, P. W. Fowler and M. V. Diudea, Patterns of counter-rotating ring currents in two valence isomers of corazulene, *Polish J. Chem.*, 2007, **81**, 653-662.
17. E. Lijnen, A. Ceulemans, M. V. Diudea and Cs. L. Nagy, Double toroids as model systems for carbon nanotube junctions: Through-bond currents, *J. Math. Chem.*, 2009, **45**, 417-430.
18. M. V. Diudea, A. E. Vizitiu, Cs. L. Nagy, T. Beu, A. Bende, and Dušana Janežič, Circulene covered fullerenes, *J. Mol. Struct. THEOCHEM*, 2009, **904**, 28-34.
19. M. V. Diudea, Counting polynomials in tori $T(4,4) S[c,n]$, *Acta Chim. Slo.*, 2010, **57**, 551-558.
20. M. V. Diudea and A. R. Ashrafi, Shell-polynomials and Cluj-Tehran index in tori $T(4,4)[5,n]$, *Acta Chim. Slo.*, 2010, **57**, 559-564.