



UNIVERSITÀ DEGLI STUDI DI MILANO

DIPARTIMENTO DI CHIMICA

Prof. Davide M. Proserpio



Davide M. Proserpio

CV January 2019

Date of birth 17 July 1962

7/1986 Laurea cum Laude at the University of Pavia (Italy) under the supervision of Prof. Luigi Fabbrizzi

12/1987-10/1989 Post Doc with Dr. Carlo Mealli at the CNR in Florence (Italy) working on applied theoretical chemistry with semiempirical calculation, developing a software for PC (see below)

11/1989 - 9/1991 Visiting Scientist in the group of the Nobel Laureate Roald Hoffmann, Cornell University NY (USA) on Applied Theoretical Chemistry using Extended Hückel calculations.

4/1992 - 11/2003 Assistant Professor at the University of Milano

12/2003 - today Associate Professor at the University of Milano (Università degli Studi di Milano, Dipartimento di Chimica)

Davide M. Proserpio in 1981 entered the "[Almo Collegio Borromeo](#)" (the oldest university college in Italy) in Pavia where started being interested in Borromeian links and got the "Laurea" in Chemistry in 1986. In the next five years he was active in the field of applied theoretical chemistry under the supervision of Dr. Carlo Mealli (CNR Florence, Italy) and spent two years with Prof. Roald Hoffmann (Nobel Laureate 1981, Cornell University, USA), developing a package for semiempirical quantum chemical calculation with the Extended Hückel approximation, called CACAO [Computer Aided Composition of Atomic Orbitals, ref [1]. The program has been quoted in the literature more than 800 times ranking the 6th most cited paper of the Journal of Chemical Education since 1961 (source Web of Science). The program is still used for a teaching and research.

In 1991 he moved to the University of Milan as assistant professor, becoming associate professor in 2003. Since his arrival at the University of Milan DMP developed a special interest on the study of the topology of crystal structures, in particular Coordination Polymers & Metal-Organic Frameworks (MOFs) [2-4] (based on covalent and coordinative bonding) and supramolecular networks [5,6] (based on weak/secondary interaction and H-bonds). The full characterization and classification of periodic structures with their nets and topological relations (entanglement, knot, interpenetration, catenation, voids) is a field of renewed interest also thanks to his contribution [7-12]. Papers [2-3] have been highly cited and are considered seminal on the study of entanglement of complex structures in particular MOFs and supramolecular architectures. Paper [2, 1792 citations] ranks 6th among the most cited papers of Coordination Chemistry Review (source Web of Science). Four papers [3,4,9,10] are among the 15 most cited papers of CrystEngComm, ranking respectively 15th, 4th, 8th and 9th in the list (source Web of Science). The field of "topological crystal chemistry" was developed also thank to the intense collaboration with Prof. Vladislav Blatov from Samara State University



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(Samara, Russia) since 2004 with the development of the software platform ToposPro used by a thousand of research around the world. The article [11] illustrating the latest development of the program has been cited already 904 times since May 2014, ranking as the most cited paper ever of Crystal Growth & Design.

In 2002 the Italian Chemical Society (SCI) awarded him with the Gold Medal Nasini for the significant contributions in Inorganic Chemistry. The “Premio Raffaello Nasini” is an award given to young scientist (less than 41th years old) for achievements in the field of Inorganic Chemistry. Was presented at the 2002 Congress of the Inorganic Chemistry Division of the Italian Chemical Society with a Lecture entitled “Coordination Polymers and Supramolecular Architectures, the new complexity of the solid state”. Award motivation: “For the outstanding results achieved in the field of Inorganic Chemistry using many different experimental and theoretical approaches that lead Dr. Proserpio to develop innovative studies on the structural chemistry of coordination polymers”

See <http://www.inorg.it/awards.html>

In 2010 the editor of Nature Chemistry asked him to write a highlight [9] on the topic of “TOPOLOGICAL CRYSTAL CHEMISTRY: Polycatenation weaves a 3D web” and in august 2011 was invited to give the prestigious Keynote Lecture at the XXII Congress of the International Union of Crystallography held in Madrid (Spain). The lecture "Topological Characterization of Coordination Networks & Metal-Organic Frameworks" was introduced by Prof. Omar Yaghi (Berkeley USA). The Keynote Lectures are awarded to prestigious scientist selected by the commissions of the IUCr. In the last Madrid conference (held every 3 years and with 2800 participants) the total number of oral presentation was 490, but only 36 were Keynote Lectures.

In 2013 won a Russian Megagrant, the most prestigious competition of the Russian Government designed to provide support to research projects implemented under the supervision of a world's leading scientist at Russian Institution of higher learning. Together with Prof. V. A. Blatov, DMP funded the Samara Center of Theoretical Material Science (www.sctms.ru; <http://english.sctms.ru>) where he is now the scientific director. The Megagrant lasted 3 years and has been renewed for two more until end of 2017.

The field of “topological crystal chemistry” was developed also thank to the intense collaboration with Prof. Vladislav Blatov from Samara State University (Samara, Russia) since 2004 and with other groups around the world, in particular: Prof. Mike O’Keeffe (Arizona State University, Tempe, AZ, USA) and Prof. Omar Yaghi (Berkeley University, CA, USA), Prof. Stephen Hyde and Dr. Olaf Delgado Friedrichs (Australian National University, Canberra, Australia), Prof. Jean-Guillaume Eon (Universidade Federal do Rio de Janeiro, Brasil).

The result of such collaborations produced since 2005 fifteen international events to introduce the “topological crystal chemistry” to young scientist and researcher from all over the world (with a total of about 400 students). The complete list is given at the bottom.

He as been invited to give numerous seminars/lectures in university and conferences in 10 different country. The list from 2001 is given at the bottom.



He is the co-author of 201 publications on international journals with referee (all indexed in the Web of Science) and 2 book chapters.

The complete list of publication with the updated citation could be examined at :
<http://www.researcherid.com/rid/C-6391-2009> (indexed by Web of Science)
<http://scholar.google.it/citations?hl=it&user=7jye64cAAAAJ> (indexed by Google Scholar)
<http://www.scopus.com/authid/detail.url?authorId=7004480576> (indexed by Scopus)

H-index = 67 (Web of Science for 17406 citations Jan. 2019) with the first publication in 1989

SELECTED REFERENCES (with citation Jan 2019):

- [1] C. Mealli, D.M. Proserpio "MO theory made visible" J. Chem. Edu. 1990, 67, 399-402 (837 cit)
- [2] L. Carlucci, G. Ciani, D.M. Proserpio "Polycatenation, polythreading and polyknotting in coordination network chemistry." Coord. Chem. Rev., 2003, 246, 247-289 (1792 cit).
- [3] L. Carlucci, G. Ciani, D.M. Proserpio "Borromean links and other non-conventional links in 'polycatenated' coordination polymers" CrystEngComm, 2003, 5, 269-279 (341 cit).
- [4] V. A. Blatov, L. Carlucci, G. Ciani, D.M. Proserpio "Interpenetrating Metal-Organic and Inorganic 3D Networks: a Computer-Aided Systematic Investigation. Part I. Analysis of the Cambridge Structural Database." CrystEngComm, 2004, 6, 377-395 (989 cit)
- [5] I.A. Baburin, V. A. Blatov, L. Carlucci, G. Ciani, D.M. Proserpio "Interpenetrated Three-Dimensional Networks of Hydrogen- Bonded Organic Species: A Systematic Analysis of the Cambridge Structural Database." Cryst. Growth Des. 2008, 8, 519. (192 cit)
- [6] I.A. Baburin, V. A. Blatov, L. Carlucci, G. Ciani, D.M. Proserpio "Interpenetrated three-dimensional hydrogen-bonded networks from metal-organic molecular and one- or two-dimensional polymeric motifs." CrystEngComm, 2008, 10, 1822-1838 (134 cit)
- [7] O. Delgado-Friedrichs, M. O'Keeffe, D.M. Proserpio, M. M. J. Treacy & O. M. Yaghi. "What do we know about three-periodic nets?" J. Solid State Chem. 2005, 178, 2533-2554 (176 cit)
- [8] D. M. Proserpio "TOPOLOGICAL CRYSTAL CHEMISTRY: Polycatenation weaves a 3D web" Nature Chemistry (2010), 2(6), 435-436. (54 cit.)
- [9] V.A. Blatov, M. O'Keeffe and D. M. Proserpio "Vertex-, face-, point-, Schläfli-, and Delaney-symbols in nets, polyhedra and tilings: recommended terminology" CrystEngComm, 2010, 12, 44-48 (499 cit)
- [10] E. V. Alexandrov, V. A. Blatov, A. V. Kochetkov and D. M. Proserpio "Underlying nets in three-periodic coordination polymers: topology, taxonomy and prediction from a computer-aided analysis of the Cambridge Structural Database" CrystEngComm, 2011, 13, 3947-3958 (418 cit.)
- [11] V.A. Blatov, A.P. Shevchenko, D.M. Proserpio "Applied Topological Analysis of Crystal Structures with the Program Package ToposPro" Cryst. Growth Des. 2014, 14, 3576-3586 (904 cit.)
- [12] L. Carlucci, G. Ciani, D. M. Proserpio, T.G. Mitina, V.A. Blatov "Entangled Two-Dimensional Coordination Networks: A General Survey" Chem. Rev. 2014, 114 (15), pp 7557-7580 (139 cit.)

INVITED LECTURES

- {26}- "Self-Assembly of Coordination Networks with Different Topology from 1,3-bis(4-pyridyl)propane and MCl₂ Salts (M = Co, Ni, Cu, Cd): Study of Properties and Monitoring of Crystallization and Interconversion Processes" 6th FIGIPS Meeting in Inorganic Chemistry - European Mediterranean Conference in Inorganic Chemistry; Barcelona, Spagna, 15-20 luglio 2001
- {27}- "Coordination Networks from the Self-Assembly of Silver Salts and the Linear Chain Dinitriles NC(CH₂)_nCN (n = 2 to 7): A Systematic Investigation of the Role of Counterions and of the Increasing Length of the Spacers" CrystEngComm Discussion 1, Innovation in Crystal Engineering, University of Bristol, UK, 1 luglio 2002
- {28}- "New polymeric architectures assembled with tetra(4-pyridyl)porphyrine building blocks" XIX Congress of the International Union of Crystallography, Ginevra, CH, 13 agosto 2002
- {29}- Seminario per il conferimento del Premio Nasini al XXX Congresso di Chimica Inorganica Modena



settembre 2002 "POLIMERI DI COORDINAZIONE E ARCHITETTURE SUPRAMOLECOLARI: aspetti strutturali e topologici ovvero la nuova complessità dello stato solido"

{30}- "Interpenetration, polycatenation, polythreading, polyknotted and more ... in coordination network chemistry" Molecular Crystal Engineering - EuroConference on Design and Preparation of Molecular Materials, Acquafredda di Maratea (PZ), 31 maggio, 5 giugno 2003

{31}- Interpenetration, polycatenation, polythreading, polyknotted in Metal Organic Frameworks" NSF Workshop on Reticular Chemistry novembre 2003 San Diego, CA USA

{32}- Interpenetration, polycatenation, polythreading, polyknotted in Metal Organic Frameworks" 3rd Italian-Korean Meeting on Inorganic Chemistry, settembre 2003, Seul, Korea

{33}- "Interpenetrating metal-organic and inorganic 3D networks: a computer-aided systematic investigation. Part I. Analysis of the Cambridge Structural Database." CrystEngComm Discussion 2 - New Trends in Crystal Engineering, University of Nottingham, UK, settembre 2004

{34}- "Topological Analysis of Interpenetrated and Polycatenated Nanoporous Materials" Arizona State University ASU, Phoenix, Arizona USA, 28 novembre 2005 su invito di M. O'Keeffe

{35}- "Topological Analysis of Interpenetrated and Polycatenated Nanoporous Materials" Universität Basel, Basel, Svizzera, 15 maggio 2006 su invito di K. Fromm

{36}- "Topological analysis of interpenetrated and polycatenated nanoporous materials" XVII Symposium of the Spanish Group of Crystallography, Sigüenza, Spagna, 13-16 giugno 2006.

{37}- "Porphyrins as building blocks for the creation of functional coordination networks" International Conference on Porphyrins and Phthalocyanines ICPP-4, Roma, 2-7 luglio 2006

{38}- "Topological analysis of interpenetrated and polycatenated nanoporous materials" Workshop on Simulation, design and crystal engineering of metal-organic frameworks presso il CECAM di Lione, Francia luglio 2007

{39}- "Graphs, nets and Tilings" meeting CHEM-MOD 2007 Chemical Graph Theory and Molecular Modeling Workshop, Università Babeş-Bolyai in Cluj Romania: ottobre 2007

{40} Lectures for the ICMR Summer School on Periodic Structures and Crystal Chemistry, University of California, Santa Barbara USA, luglio 2008

{41} - "Topological analysis of Interpenetrated and polycatenated nanoporous materials" Nanotechnology International Forum, Rusnanoforum, Mosca (Russia), dicembre 2008.

{42} Lectures for "Summer Schools on Mathematical Crystallography" Nancy, France, 21 June - 2 July 2010 (con V.A. Blatov)

{43} Lectures for "Computer methods in crystal structure systematics" Max Planck Institute for Solid State Research, Stuttgart, Germany, settembre 2011

{44} - "Topological crystal chemistry: nets and entanglements in periodic structures" Topological Dynamics in Physics and Biology, July 12 - 13, 2011, presso il Centro di Ricerca Matematica Ennio de Giorgi, Pisa, luglio 2011

{45}- "Topological Characterization of Coordination Networks & Metal Metal-Organic Frameworks" Keynote Lecture, XXII Congress of the International Union of Crystallography (IUCr) Madrid (Spagna) 22-30 agosto 2011

{46} - "Topological crystal chemistry: nets and entanglements in periodic structures" Special Session on Modeling Crystalline and Quasi-Crystalline Materials all' AMS (America Mathematical Society) Section Meeting in Tampa (Florida - USA), 10-11 Marzo 2012

{47} - "From Eutax to Topos following Mike's path." Meeting: "Beautiful crystals for the world - A celebration of Michael O'Keeffe's half a century of contributions to symmetry and patterns in chemistry". Purbeck House Hotel, 91 High Street, Swanage, Dorset, UK, 3-4 maggio 2012.

{48} - Lectures for Summer School "Computer Topological Analysis of Molecular Crystals and Coordination Networks" organizzata dalla Universidad Internacional Menéndez Pelayo (Santander, Spagna), luglio 2012.

{49} - "Topological crystal chemistry: nets and entanglements in periodic structures" meeting: SMARTER 3 (Structure elucidation by combining Magnetic Resonance, computation modeling and diffractions.) University of Versailles Saint-Quentin-en-Yvelines (France), 10-13 settembre 2012.

{50} - "Periodic Structures and Crystal Chemistry: A history of the topological approach to crystal chemistry by means of the cds net." Universidade Federal do Rio de Janeiro, Brasil, 7 November 2013.

{51} - "Topological Characterization of Coordination Networks & Metal-Organic Frameworks : nets and entanglements in periodic structures". Gordon Research Conference: Crystal Engineering. Waterville Valley Resort - USA, 2 June 2014.



- {52} - "The nanocluster approach to elucidate complex intermetallics" SCTE 2014, 19th International Conference on Solid Compounds of Transition Elements, Genova, Italia, 26 June 2014
- {53} - "ToposPros: an introduction with practical examples" 1st European Crystallographic School, Pavia, Italia. 5 September 2014
- {54} - "Periodic Structures and Crystal Chemistry: A history of the topological approach to crystal chemistry by means of the cds net." Associazione Italiana di Cristallografia: 2nd Joint AIC-SILS conference. Firenze, Italia. 18 September 2014
- {55} - "Topological methods in crystal chemistry and materials science" 1st International Scientific Conference: Science of the future, San Petersburg, Russia. 19 September 2014
- {56} - "Entanglement in 2-periodic coordination networks". "150 Years of Beautiful Structures and Defects" a Symposium to honor Prof. Mike O'Keefe and Prof. Osamu Terasaki. Ho-Chi Min City, Vietnam. 15 November 2014
- {57} - "Crystal structure topology as a key for materials design", Meeting organized by Prof. Artem R. Oganov on "New Approaches in Materials Design", Moscow, Russia, 11 December 2014
- {58} - "Periodic Structures and Crystal Chemistry: A history of the topological approach to crystal chemistry by means of the cds net." Technische Universitaet Dresden, Institut fuer Physikalische Chemie, Dresden, Germany. 13 April 2015
- {59} - "Entanglements: old and new views" IUPAC project meeting and workshop: "Topology representations in coordination networks, metal-organic frameworks and other crystalline materials" Samara Center for Theoretical Materials Science, Samara, Russia. May 21-23, 2015
- {60} - "The nanocluster approach to elucidate complex intermetallics" ECM-29 European Crystallographic Meeting. Rovinj, Croatia. 23-28 August 2015
- {61} - "Entanglement in 2-Periodic Coordination Networks" Conference of the Soc. for Industrial and Appl. Mathematics (SIAM). Session on Mathematical Aspects of Materials Science. Philadelphia, USA. 9 May 2016
- {62} - "Periodic Structures and Crystal Chemistry." Invited by Prof. Jing Li, Rutgers University, Piscataway, USA. 10 May 2016
- {63} - "Carbon allotropes database" Workshop iPolymorphs: novel routes to inorganic polymorphs Science. Donostia, Spain. 23 June 2016
- {64} - "Periodic structures and crystal chemistry" 2nd International Scientific Conference: Science of the future, Kazan, Russia. 20-23 September 2016
- {65} - "Hands on ToposPro" invited by Prof. Berend Smit at the Laboratory of Molecular Simulation LSMO, École Polytechnique Fédérale de Lausanne EPFL, Sion, Switzerland. 22 May 2017
- {66} - "Exploring structural space searching for carbon allotropes" ACNS'2017, 13th International Conference on Advanced Carbon NanoStructures, Saint Petersburg, Russia. July 3-7, 2017.
- {67} - "Exploring structural space searching for carbon allotropes" 254th National Meeting and Exposition of the American Chemical Society, Washington DC, USA. August 20-24, 2017
- {68} - "Topological characterization of coordination networks and MOFs" and "Hands on ToposPro" at IWSN-2017 International school for young researchers "Smart Nanomaterials" Rostov-on-Don, Russia. September 11-15, 2017
- {69} - "Perchè citiamo? L'etica delle citazioni e gli (ipotetici) allotropi del carbonio" Nanolab Talk, Dipartimento di Energia, Cesnef, Politecnico di Milano. 9 April 2018



International Schools/Courses/Workshops

1. "Topology of crystal structures: nets, knots and surfaces" IUCr-XX congress, Microsymposium 66 - Firenze, August 2005. <http://xxiucr.iccom.cnr.it/ms66.htm>
<http://www.crystallography.fr/mathcryst/iucrXX-ms66.php>
2. "Theoretical Aspects of Design of Periodic Materials" CECAM workshop, Lyon (France), July 2007 (with M. O'Keeffe) 47 participants from 15 countries. <http://www.cecama.org/workshop-155.html>
3. "ICMR Summer School on Periodic Structures and Crystal Chemistry", University of California, Santa Barbara USA, July 2008, (with M. O'Keeffe) with 36 students from 12 countries. <http://www.icmr.ucsb.edu/programs/archive/crystalchemistry.html>
4. "Summer Schools on Mathematical Crystallography" Nancy, France, 21 June - 2 July 2010 (with V.A. Blatov) with 47 students from 17 countries. <http://www.crystallography.fr/mathcryst/nancy2010.php>
5. "Computer methods in crystal structure systematics" September 19-22, 2011 Max Planck Institute for Solid State Research, Stuttgart, Germany (with V.A. Blatov) with 36 students from 7 countries <http://www.fkf.mpg.de/xray/>
6. One day course introduction to TOPOS, Invited by Prof. M. Zaworotko, Departement of Chemistry, University of South Florida (USF), Tampa, FL, USA, March 9, 2012. With 12 students.
7. Summer School "Computer Topological Analysis of Molecular Crystals and Coordination Networks" organized by the Universidad Internacional Menéndez Pelayo (Santander, Spain) July 16-18, 2012, with 23 PhD students and 4 professor from 4 countries. <http://www.topos.samsu.ru/Santander.html>
8. School on "Computer topological analysis of MOFs and coordination networks" (with M. O'Keeffe). Lawrence Berkeley National Lab (California, USA), on 4-7 February 2013. withr 25 students from groups of Berkely University (Omar Yaghi, Jeffrey Long) and Texas A&M (Zhou).
9. School on "Topological methods in crystal chemistry and materials science" (with V.A. Blatov). CECAM-HQ-EPFL, Lausanne, Switzerland. September 9-13, 2013. For 40 partecipants. <http://www.cecama.org/workshop-869.html>
10. School on "Topological methods for expert systems in Material Science" (with V.A. Blatov) Samara, Russia. 3-7 February 2014. See <http://english.sctms.ru/training/school/>
11. School on "Topological methods for expert systems in Material Science" (with V.A. Blatov) Samara, Russia, 12-16 August 2014. See <http://english.sctms.ru/training/school/>
12. International Conference "Bridging the Gap between Solid State Quantum Chemistry and Structural Chemistry of Allotropes": The 14th Session of the V.A. Fock meeting on quantum and Computational Chemistry. Samara, Russia. 18-22 August 2014. See: <http://english.sctms.ru/training/conference/>
13. IUPAC project meeting and workshop: "Topology representations in coordination networks, metal-organic frameworks and other crystalline materials» Samara Center for Theoretical Materials Science, Samara, Russia. May 21-23, 2015. See: http://english.sctms.ru/novosti_centra/20150619_01/
14. School on "Combined Topological and DFT Methods for Prediction of New Materials" (with V.A. Blatov) Samara, Russia, 15-20 September 2015. See <http://english.sctms.ru/training/school/>
15. School on "Combined Topological and DFT Methods for Prediction of New Materials II" (with V.A. Blatov) Samara, Russia, 4-10 July 2016. See <http://english.sctms.ru/training/school/>