



UNIVERSITÀ DEGLI STUDI DI MILANO

DIPARTIMENTO DI CHIMICA

Prof. Davide M. Proserpio



Davide M. Proserpio

CV october 2013

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 Borromean 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 first 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 then D.M. Proserpio 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 [7,8]. Papers [2-3] have been highly cited and are considered seminal on the study of entanglement of complex structures in particular new materials such MOFs. Paper [2] ranks 3rd as the most cited paper of Coordination Chemistry Review (source Web of Science). Moreover [4], on the topology of interpenetration, was highlighted in February 2006 as a Fast Breaking Paper by ISI Essential Science Indicators Web Product ESI (see http://www.esi-topics.com/fbp/2006/february06-Blatov_Proserpio.html). Both ref 3 and 4 are among the 10 most cited papers of CrystEngComm, ranking 3rd and 8th in the list (source Web of Science).



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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://dci.mfn.unipmn.it/premi_it.html#nasini

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.

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 nine international events to introduce the "topological crystal chemistry" to young scientist and researcher from all over the world (with a total of about 200 students). The complete list is given at the bottom.

He as been invited to give numerous seminars/lectures in university and conferences in 9 different country. The complete list is given at the bottom.

He is the co-author of 155 publications (+ 3 in press) 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)

or at the page indexed by Google Scholar:

<http://scholar.google.it/citations?hl=it&user=7jye64cAAAAJ>

H-index = 56 (Web of Science for 10998 citations october 2013) with the first publication in 1989



REFERENCES (with citation jan. 2013):

- [1] C. Mealli, D.M. Proserpio "MO theory made visible" *J. Chem. Edu.* 1990, 67, 399-402 (812 cit)
- [2] L. Carlucci, G. Ciani, D.M. Proserpio "Polycatenation, polythreading and polyknotting in coordination network chemistry." *Coord. Chem. Rev.*, 2003, 246, 247-289 (1270 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 (267 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 (440 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. (130 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 (82 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 (103 cit)
- [8] Chapter 1.3 pag 58-85 on "Networks, Topologies and Entanglements" by L. Carlucci, G. Ciani and D. M. Proserpio in "Making Crystals by Design. Methods, Techniques and Applications" Wiley, 2007, edited by D. Braga and F. Grepioni (35 cit)
- [9] D. M. Proserpio "TOPOLOGICAL CRYSTAL CHEMISTRY: Polycatenation weaves a 3D web" *Nature Chemistry* (2010), 2(6), 435-436. (22 cit.)

INVITED LECTURES

- {1}- "Molecular Mechanism of Photosynthetic Oxygen Evolution: A Theoretical Approach " 2nd Italian-Portuguese-Spanish Meeting in Inorganic Chemistry, Alfa Mar, Algarve, Portugal, 23-27 March 1992
- {2}- "Calcoli di Orbitale Molecolare con il metodo Extended Hückel" Scuola della Associazione Italiana di Cristallografia, Perugia, 14-18 Settembre 1992 "Qualitative Molecular Orbital Theory on a PC using the CACAO Programs"
- {3}- University College Dublin, Dept. of Chemistry, 24 Novembre 1992
- {4}- University of Dortmund, Germany, Dept. of Inorganic Chemistry, 27 Aprile 1993
- {5}- University of Hannover, Germany, Inst. of Inorganic Chemistry, 29 Aprile 1993
- {6}- Max-Planck-Institut fuer Festkörperforschung, Stuttgart, Germany, 3 Maggio 1993
- {7}- University of Bern, Switzerland, Dept. of Inorganic and Physical Chemistry, 5 Maggio 1993
- {8}- University of Lausanne, Switzerland, Inst. of Inorganic and Analytical Chemistry, 6 Maggio 1993
- {9}- "Extended Huckel Theory at work: Transition Metal Clusters" European Science Foundation Workshop: Theoretical Aspects of Cluster Chemistry, Isle of Thorns, Chelwood Gate, Sussex, England, 16-19 Luglio 1994
- {10}- "Theoretical Modeling of the Mechanism of Dioxygen Activation by Tetranuclear Manganese Complexes" 10th International Conference on Photochemical Conversion and Storage of Solar Energy, Interlaken, Switzerland, 25-29 Luglio 1994, Abstract p. 49-50
- {11}- "CACAO (Computer Aided Composition of Atomic Orbitals). An Interactive Package of Programs for Molecular Orbital Analysis" 208th American Chemical Society National Meeting, Washington DC, USA, 21-25 Agosto 1994 Division of Computers in Chemistry, Abstract COMP042
- {12}- "Use and Application of Extended Hückel Methods" EXXON, Annandale, NJ, USA, 29 Agosto 1994
- {13}- "Theoretical Modeling of the Mechanism of Dioxygen Activation by Tetranuclear Manganese Complexes" European Science Foundation Workshop: The Oxygen Evolving Enzyme, Gif-sur-Yvette, France, 6-9 Novembre 1994 "Silver Polymeric Networks: a World of Structures and Topology"
- {14}- University of Köln, Germany, Inst. of Inorganic Chemistry, 19 Novembre 1997
- {15}- University of Bonn, Germany, Inst. of Inorganic Chemistry, 20 Novembre 1997
- {16}- Aachen University of Technology, Germany, Inst. of Inorganic Chemistry, 21 Novembre 1997



- {17}- "New Topological Types and Intertwined Motifs in Coordination Polymers Assembled with Long Bidentate N-Donor Ligands" XXVI Congresso Nazionale di Chimica Inorganica, Acquafredda di Maratea (PZ), 1 luglio 1998 "Polymeric Networks: a World of Structures and Topology"
- {18}- Sichuan Union University, Chengdu, Sichuan, China, Dept. of Chemistry, 19 Maggio 1999
- {19}- GuangXi University, Nanning, GuangXi, China, Dept. of Chemistry, 31 Maggio 1999
- {20}- Peking University, Beijing, China, Dept. of Chemistry, 4 Giugno 1999 "Qualitative Molecular Orbital Theory on a PC using the CACAO Programs"
- {21}- Sichuan Union University, Chengdu, Sichuan, China, Dept. of Chemistry, 19 Maggio 1999
- {22}- GuangXi University, Nanning, GuangXi, China, Dept. of Chemistry, 31 Maggio 1999
- {23}- " Coordination Networks: a World of Structures and Topology" University of California, Berkeley, USA, Dep. of Chemistry, Special Inorganic Seminar, 28 Agosto 2000
- {24}- " New Examples of Self-Catenation in two Three-Dimensional Polymeric Co-Ordination Networks" Dalton Discussion 3, Inorganic Crystal Engineering, Università di Bologna, 10 settembre 2000.
- {25}- "Novel Nanoporous Coordination Frameworks Assembled with non-Rigid Bidentate Pyridyl Ligands" XXX Congresso Nazionale della Ass. Italiana di Cristallografia Martina Franca, 22 settembre 2000
- {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, polyknotting 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, polyknotting in Metal Organic Frameworks" NSF Workshop on Reticular Chemistry novembre 2003 San Diego, CA USA
- {32}- Interpenetration, polycatenation, polythreading, polyknotting 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 Ia 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 coMbinig mAgnetic Resonance, compuTation modELing and diffRactions.) University of Versailles Saint-Quentin-en-Yvelines (France), 10-13 settembre 2012.

Organizer of 9 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.cecarn.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. with 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 participants. <http://www.cecarn.org/workshop-869.html>