

Leonardo Lo Presti

CURRICULUM VITAE

Updated March, 2019

General indicators

Researcher ID: K-4281-2012

ORCID: orcid.org/0000-0001-6361-477X

ResearchGate: https://www.researchgate.net/profile/Leonardo_Lo_Presti

Google Scholar: <https://scholar.google.it/citations?hl=it&user=8XpBy48AAAAJ>

In service from (Department of Chemistry) **01/09/2007**

Number of papers in the last 5 years (2014-2019): **39**

Total number of papers (2002-2019): **68**

Book Chapters: **2**

H-Index (WoS): 17

H-Index (Scopus): 17

H-Index (Google Scholar): 18

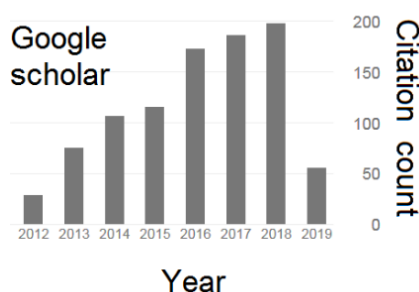
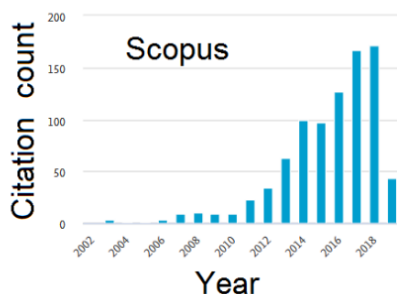
i-10 Index (Google Scholar): 42

i-10 Index: (Google Scholar): 32

Total citations (WoS): 825

Total citations (Scopus): 874

Total citations (Google Scholar): 1033



Research Gate Score: 45.3 (> 97.5 % RG percentile)

Research activity

My research interests concerns the following topics.

- (i) Development of predictive theories of the solid state applied to organic molecular crystals. At the moment, the most successful methods for crystal structure prediction are based on "brute-force" approaches: a large number of possible structure is simulated and screened to look for the most cohesive energies. This line of research has the ambition to look for correlations between the collective thermodynamic properties of the molecular ensemble out of equilibrium and the symmetry in the resulting crystal. To this end, classical Molecular Dynamics and Monte Carlo techniques are applied to the simulation of liquids, solutions and nano-aggregates, coupled with statistical data mining techniques applied to crystallographic databases. Also closely related to this argument is the study of the correlations between the electron density and the crystal field.

- (ii) Study of 4-aminoquinoline antimalarials as inhibitors of crystallization of hematin, a crucial step of the metabolism of Plasmodium. The idea of the present study is to investigate how the 4-aminoquinoline drug interacts with its substrate, free heme, to design chemical modifications to improve its activity.
- (iii) Structure-property correlations in advanced materials. By coupling experimental techniques (powder X-ray diffraction, X-ray absorption spectroscopy) and computational tools (quantum simulations in the solid or surface), it is possible to study the interplay between the structure of the material at various length scales and to determine how and why specific intensive properties emerge at the macroscale. In particular, I am now studying TiO₂-based nanostructured photocatalysts for environmental remediation, correlations between crystal structure and nonlinear optical properties in metal-organic frameworks with teranostic applications, and correlations between structural phase transitions and ferroelectric properties in perovskites of Ta / Nb for advanced photonic applications.

Until March 2019, I produced 68 articles in peer-reviewed journals, 2 book chapters and more than 40 oral and poster communications at national and international conferences. The detailed list of publications is shown at the end of this CV (from page 6).

I qualified for the functions of Associate Professor in the SSD 03 / A2 (MODELS AND METHODOLOGIES FOR CHEMICAL SCIENCES, from 10/04/2017 to 10/04/2023, call 2016 first quarter) and 03 / B1 (FUNDAMENTALS OF CHEMICAL SCIENCES AND INORGANIC SYSTEMS, from 12/04/2017 to 04/12/2023, call 2016 first quarter).

Funding

I won a total of 12 between national and international competitive funding as Principal Investigator (out of a total of 18 funded projects) to get beamtime at synchrotron / neutron sources and high-performance computational resources. All the projects were evaluated by anonymous experts according to usual blind peer review practices. In addition, I won 2 local grants in the context of the "Development Plan" of Università degli Studi di Milano for supporting scientific excellences. I also participated to PUR 2008 project, and I was the PI of a PUR 10% (2009). In 2018 I won a grant related to the Annual Fund for Basic Research Activities (FFABR) of the Italian Ministry of High Education. Overall, I was the Principal Investigator of 16 (~ 70 %) funded projects. Five doctoral scholarships were also activated under my responsibility, which are completely paid by the Center for Materials Crystallography in Århus through the Italian CNR.

Participation to International Centres and Editorial Boards

- (i) From 2010 I am associated (<http://chem.au.dk/forskning/forskningscentre/center-for-materials-crystallography/about-cmc/staff/>, see "Partners") to the Center for Materials Crystallography (CMC) in Århus (DK), which completely funded 5 PhD positions of the Doctoral School in Chemistry at Università degli Studi di Milano.
- (ii) From 25/03/2011 to 25/11/2014 I was associated to the Institute of Molecular Sciences and Technologies of the Italian National Research Council (CNR) to carry out a project on the analysis of experimental charge density distributions with advanced computational and experimental tools.
- (iii) From 22/07/2017 to 21/07/2019, I am associated again to ISTM-CNR to carry out the following project: "*Experimental and theoretical study of correlated materials of potential chemical and technological interest*".
- (iv) Since 2007, I joined the Italian Crystallographic Association (AIC, <http://www.cristallografia.org/>), a no-profit organization that aims to promote crystallography in all its educational and scientific aspects.
- (v) I am currently Guest Editor for a special issue of the open access journal "Crystals" (Impact Factor = 2.144) dedicated to gel crystallization methods or gel-like systems

http://www.mdpi.com/journal/crystals/special_issues/Crystal_Growth_Gels).

Awards

- As an undergraduate student, 100% exemption of tuition fees for curricular merits.
- Winner of a doctoral scholarship for the Chemistry school (2000-2003).
- Winner of a two-year research grant, renewed once, at the Department of Physical Chemistry and Electrochemistry of the University of Milan (2003-2007).
- National Award of the Italian Association of Crystallography (AIC) for the best master thesis in crystallography: "Experimental and Theoretical Study of the Mechanism of Action of the Chloroquine Antimalarial Drug" presented by my master student Giovanni Macetti. This thesis work subsequently produced two scientific publications (DOI: 10.1088 / 0031-8949 / 91/2/023001; DOI: 10.1021 / acs.cgd.6b01069).
- National Award of the Italian Association of Crystallography (AIC) for the best master thesis in crystallography: "Correlations among solubility and crystal structure: a crystallographic and spectroscopic study of the antimalarial drug piperazine" presented by my master student Pietro Sacchi. This thesis work has already produced a scientific publication (DOI: 10.1021 / acs.cgd.8b01794).
- Other awards:
Invited papers.
 - o New Talent themed issue per **CrystEngComm**, 2018 (DOI: 10.1039/C8CE00674A)
 - o Margaret C. (Peggy) Etter Virtual Memorial Issue per **Crystal Growth & Design**, 2016 (DOI: 10.1021/acs.cgd.5b00442).
 - o Focus issue on Charge, Spin and Momentum Densities: SAGAMORE XVIII per **Physica Scripta**, 2016 (DOI: 10.1088/0031-8949/91/2/023001)

Participation as a speaker at congresses and conferences of international interest

I present **22 oral communications** at international congresses e workshops (6 invited). I was the presenting person in **7 talks**. I also presented **24 poster**. **5 contributions** were published as "*Conference Papers*" in appendix to Acta Crystallographica Section A: Foundations of Crystallography.

Organization of International Congresses

- ICG2017 - Italian Crystal Growth Conference, Milano (Italy), 20-21/11/2017 (Co-chair) (<http://cristallografia.org/contenuto/icg2017--first-circular/2941>)
- SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities, S. Margherita di Pula (CA), Italy, 7-12/06/2015 (Comitato organizzatore) (<http://www.sagamorexviii.org/>)
- ECDM-5 *European Charge Density Meeting*, Gravedona (CO), Italy, 6-11/06/2008 (Comitato organizzatore) (<http://ecdm5.istm.cnr.it/>)

Peer-review activity

I performed more than 90 peer-reviews, including first submissions and resubmissions, mainly for the following international journals: Advanced Materials, Scientific Reports, Chemistry - A European Journal, Physical Chemistry Chemical Physics, Journal of Physical Chemistry, Inorganic Chemistry, Dalton Transactions, Acta Crystallographica, Solar Energy Materials and Solar Cells, Journal of Molecular Structure, Materials Chemistry, Materials Chemistry Frontiers, Materials Chemistry and Physics, Journal of American Ceramic Society, Powder Diffraction Journal, International Journal of Modern Physics.

I also performed invited evaluations of international competitive projects for the following funding agencies: **National Science Foundation (USA)** and **Austrian Science Fund (FWF)**.

Teaching, supplementary teaching and student service activities

Frontal lessons

- (1) 2008-present: MSc in Chemical Sciences: **Crystal Chemistry** (6 ECTS).
- (2) 2012-present. BSc in Chemistry: **Chemical Physics Methods for the investigation of Molecular and Nanostructured Systems** (3 ECTS).
- (3) 2016-present: MSc in Molecular Biotechnologies and Bioinformatics: **Rational design and structural characterization of bioactive molecules** (3 ECTS).
- (4) 2014-2015: MSc in Molecular Biotechnologies and Bioinformatics: **Advanced chemical methods applied to Biotechnologies** (3 ECTS).
- (5) 2008-2013: MSc in Molecular Biotechnologies and Bioinformatics: **Mathematical, Physical and Chemical Methods applied to Biotechnologies** (3 ECTS).
- (5) 2008-2010: BSc in Biology: **General Chemistry with Physical Chemistry** (1 ECTS of exercises).

Laboratory Assistance

- (1) **2008-2010** and **2013-present**: BSc in Chemistry: **Physical Chemistry 1**.
- (2) **2011-2012**: BSc in Chemistry: **Physical Chemistry 2**.
- (3) **2008-2010**: MSc in Chemical Sciences: **Physical Chemistry B**.

Tutoring

In 2010-2013 e 2017-present I have carried out, and I am still doing, non-disciplinary tutoring activities for the BSc students in Chemistry.

PhD courses

- (1) May 2013: **Coordinator**, with prof. Michele Ceotto, of the PhD course on "*Taking a glance on ultrasmall and ultrafast worlds: time-resolved and free electron laser probes for chemical applications*" (PhD in Chemistry)
 - 2 lectures (4 hrs): Dr. Leonardo Lo Presti, Università degli Studi di Milano;
 - 2 lectures (4 hrs): Prof. Michele Ceotto, Università degli Studi di Milano;
 - 2 lectures (4 hrs): Invited speaker: Prof. Jan Davidsson, Uppsala Universitet
- (2) March 2015: Lecture (2 hrs) on "*Diffraction and EXAFS methods*" for the PhD course on "*Physical Chemistry of Nanosized Titania: first principles calculations vs. experiments*" (PhD in Chemistry)
- (3) June 2015: Lecture (2 hrs) on "*Encoding and decoding crystal structures*" for the PhD course on '*From Molecules to Crystals*' (PhD in Chemistry)
- (4) May-June 2017: **Coordinator** of the PhD course on "*Discovering molecular recognition and self-assembling through the lenses of non-covalent interactions*" (PhD in Chemistry)
 - 2 lectures (4 hrs): Dr. Leonardo Lo Presti, Università degli Studi di Milano;
 - 1 lecture (2 hrs): Dr. Stefano Pieraccini, Università degli Studi di Milano;
 - 1 lecture (2 hrs): Dr. Alessandra Forni, CNR-ISTM

- 1 lecture (2 hrs): Prof. Giancarlo Terraneo, Politecnico di Milano
- (5) July, 2019: **Coordinator** of the PhD course on “*Making experiment and theory talking together: A multidisciplinary approach for materials science*” (PhD in Chemistry)
- 1 lecture (2 hrs): Dr. Leonardo Lo Presti, Università degli Studi di Milano;
 - 1 lecture (2 hrs): Prof. Marco Merlini, Università degli Studi di Milano;
 - 1 lecture (2 hrs): Prof. Matteo Alvaro, Università degli Studi di Pavia;
 - 1 lecture (2 hrs): Dr. Guido Sello, Università degli Studi di Milano;
 - 1 lecture (2 hrs): Prof. Roberto Todeschini e Prof. Davide Ballabio, Università degli Studi di Milano-Bicocca

PhD, MSc and BSc students

- From 2008 to 2019 I was the supervisor of **15 MSc** and **5 BSc**.
- I supervised 5 PhD students entirely funded by CMC in Århus.

Third Mission and Orientation

- (1) 2011-2013. “Energy Lab”. This initiative involved **10 secondary schools** and almost **400 secondary school students**.
- (2) 2011-2014. Coordination of the Physical Chemistry part of the interdisciplinary **Summer School “Marinella Ferrari”**, addressed at secondary school students.
- (3) March 2012: Stand set up at the **Civic Aquarium of Milano** on the occasion of the initiative “interactive chemistry laboratories” organized in the context of “The Adventure of Science”, with practical demonstration on the energy conversion.
- (4) February-May 2014: “*Crystals*” demonstration on the occasion of the initiative “**Under 18 Science**” addressed at secondary school students.
- (5) May, 10th 2014: “*Unimi Under 18*” event: stand set up, where young students showed the crystals grown by themselves in their own schools.
- (6) June 2014: Organization of the presentation ceremony of the “*Crystals in Unimi*” exhibition
- (7) June 2014. Preparation of the “*Crystals in Unimi*” exhibition, organized within the initiatives of the Italian Crystallographic Association in the context of the celebrations for the International Year of Crystallography.
- (8) November, 28th 2014. Dissemination Seminar: “*Signals from the invisible: a brief history of diffraction*”, presented at the Civic Museum of Natural History in Milan under the patronage of the Lombard Mineralogical Group - Italian Association of Mineralogy, as part of the initiatives for the International Year of Crystallography.
- (9) 27 febbraio 2015: Dissemination Seminar “*Brief introduction to crystallography*” in the context of **Progetto Lauree Scientifiche (PLS)** initiative
- (10) May 19th, 2017. Dissemination Seminar “*Signals from the invisible: a brief history of diffraction*”, presented at the Auditorium Levi in Milan as part of the PLS event “Waves, Minerals and Crystals: History and Applications”.

Institutional, organizational and service activities

- 2008-2009; 2013-present: **Teaching Board** of the PhD school in Chemistry.
- 2018-present: **Taching Commission** of the Chemistry Department.
- 2018-present: **Coordinator of the Commission for Instrumentation and Technical Gases**.
- 2017-present: **Committee for the access to the Master Degrees**.

- 2012-2018: Commission for Instrumentation and Technical Gases.
 - 2012-2016: Secretary of the Parithetic Commission.
 - 2011-2015: Orientation Committee.
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Scientific papers.

- (A1) Domenica Marabello*, Paola Antoniotti, Paola Benzi, Elena Cariati, **Leonardo Lo Presti**, Carlo Canepa: *Developing new SrI_2 and β -D-fructopyranose-based metal-organic frameworks with nonlinear optical properties*. Acta Crystallographica Section B75 2019, *In press*. DOI: 10.1107/S2052520619001951
- (A2) Pietro Sacchi, Laura Loconte, Giovanni Macetti, Silvia Rizzato*, **Leonardo Lo Presti***: *Correlations of Crystal Structure and Solubility in Organic Salts: The Case of the Antiplasmodial Drug Pipleraquine*. Cryst. Growth Des. 2019, 19, 1399-1410, DOI: 10.1021/acs.cgd.8b01794
- (A3) Angelo Gavezzotti*, **Leonardo Lo Presti**: *Dynamic simulation of liquid molecular nanoclusters. Structure, stability and quantification of internal (pseudo)symmetries*. New J. Chem., 2019,43, 2077-2084, DOI: 10.1039/C8NJ05825C
- (A4) Andrea Gionda, Giovanni Macetti, Laura Loconte, Silvia Rizzato, Ahmed M. Orlando, Carlo Gatti, **Leonardo Lo Presti***: *A variable-temperature X-ray diffraction and theoretical study of conformational polymorphism in a complex organic molecule (DTC)*. RSC Adv., 2018,8, 38445-38454. DOI: 10.1039/C8RA08063A
- (A5) Luca Carlino, Michael Christodoulou, Valentina Restelli, Fabiana Caporuscio, Francesca Foschi, Marta S. Semrau, Elisa Costanzi, Annachiara Tinivella, Luca Pinzi, **Leonardo Lo Presti**, Roberto Battistutta, Paola Storici, Massimo Broggin, Daniele Passarella*: *Structure-Activity Relationships of Hexahydrocyclopenta[c]quinoline Derivatives as Allosteric Inhibitors of CDK2 and EGFR*. ChemMedChem 2018, 13, 2627-2634, DOI: 10.1002/cmdc.201800687
- (A6) Angelo Gavezzotti, Silvia Rizzato, **Leonardo Lo Presti***: *The TACO Puzzle: A Phase-Transition Mystery Revisited*. Crystal Growth & Design 2018, 18, 7219-7227, DOI: 10.1021/acs.cgd.8b01461
- (A7) Giulia Rainoldi, Giordano Lesma, Claudia Picozzi, **Leonardo Lo Presti**, Alessandra Silvani*: *One step access to oxindole-based β -lactams through Ugi four-center three-component reaction*. RSC Advances 2018, 8, 34903-34910, DOI: 10.1039/C8RA08165D
- (A8) **Leonardo Lo Presti***: *On the significance of weak hydrogen bonds in crystal packing: a large databank comparison of polymorphic structures*. CrystEngComm, 2018, 20, 5976-5989, DOI: 10.1039/C8CE00674A (invited paper for the 2018 "New talent" themed issue)
- (A9) Silvia Rizzato*, Massimo Moret*, Fabio Beghi, **Leonardo Lo Presti**: *Crystallization and structural properties of a family of isotopological 3D-networks: the case of 4,4'-bipy ligand - M^{2+} triflate system*. CrystEngComm, 2018,20, 3784-3795. DOI: 10.1039/C8CE00653
- (A10) Cinzia Colombo*, Ārtomir Podlipnik, **Leonardo Lo Presti**, Masahiro Niikura, Andrew J. Bennet, Anna Bernardi: *Design and synthesis of constrained bicyclic molecules as candidate inhibitors of influenza A neuraminidase*. PLoS ONE, 2018, 13(2) e0193623, 1 - 22, DOI: 10.1371/journal.pone.0193623
- (A11) Giulia Rainoldi*, Fabio Begnini, Mariska de Munnik, **Leonardo Lo Presti**, Christophe M. L. Vande Velde, Romano Orru, Giordano Lesma, Eelco Ruijter, Alessandra Silvani: *Sequential Multicomponent Strategy for the Diastereoselective Synthesis of Densely Functionalized Spirooxindole-Fused Thiazolidines*. ACS Combinatorial Science, 2018, 20 (2), 98-105, DOI: 10.1021/acscmbosci.7b00179 (
- (A12) Giovanni Macetti, **Leonardo Lo Presti**, Carlo Gatti*: *Spin density accuracy and distribution in azido Cu(II) complexes: A source function analysis*. Journal of Computational Chemistry, 2018, 39(10), 587-603, DOI: 10.1002/jcc.25150
- (A13) Lucia Tamborini, Federica Mastronardi, **Leonardo Lo Presti**, Birgitte Nielsen, Carlo De Micheli, Paola Conti, Andrea Pinto*: *Synthesis of l-Tricholomic Acid Analogues and Pharmacological*

Characterization at Ionotropic Glutamate Receptors. ChemistrySelect 2017, 2(31):10295-10299, DOI: 10.1002/slct.201702154

- (A14) Giovanni Di Liberto, Valentina Pifferi, **Leonardo Lo Presti***, Michele Ceotto*, Luigi Falciola*: *Atomistic Explanation for Interlayer Charge Transfer in Metal-Semiconductor Nanocomposites: The Case of Silver and Anatase*. Journal of Physical Chemistry Letters 10/2017, 8, 5372-5377, DOI: 10.1021/acs.jpcclett.7b02555
- (A15) Riccardo Destro*, Riccardo Ruffo, Pietro Roversi, Raffaella Soave, Laura Loconte, **Leonardo Lo Presti**: *Anharmonic motions versus dynamic disorder at the Mg ion from the charge densities in pyrope (Mg₃Al₂Si₃O₁₂) crystals at 30 K: Six of one, half a dozen of the other*. Acta Crystallographica Section B: Structural Science, 04/2017; 73, 722-736, DOI: 10.1107/S2052520617006102
- (A16) Carlo Gatti*, Giovanni Macetti, **Leonardo Lo Presti**: *Insights on spin delocalization and spin polarization mechanisms in crystals of azido copper(II) dinuclear complexes through the electron spin density Source Function*. Acta Crystallographica Section B: Structural Science, 08/2017, 73(4):565-583, DOI: 10.1107/S2052520617008083
- (A17) Valentina Colombo, **Leonardo Lo Presti***, Angelo Gavezzotti: *Two-component organic crystals without hydrogen bonding: structure and intermolecular interaction in bimolecular stacking*. CrystEngComm 03/2017; 19:2413-2423., DOI:10.1039/C7CE00311K
- (A18) Daniela Meroni*, **Leonardo Lo Presti***, Giovanni Di Liberto, Michele Ceotto, Robert G Acres, Kevin C Prince, Roberto Bellani, Guido Soliveri, Silvia Ardizzone: *A Close Look at the Structure of the TiO₂-APTES Interface in Hybrid Nanomaterials and Its Degradation Pathway: An Experimental and Theoretical Study*. The Journal of Physical Chemistry C 01/2017; 121:430-440., DOI:10.1021/acs.jpcc.6b10720
- (A19) Michael S Christodoulou, Fabiana Caporuscio, Valentina Restelli, Luca Carlino, Giuseppe Cannazza, Elisa Costanzi, Cinzia Citti, **Leonardo Lo Presti**, Pasquale Pisani, Roberto Battistutta, Massimo Broggin, Daniele Passarella, Giulio Rastelli*: *Probing an Allosteric Pocket of CDK2 with Small Molecules*. ChemMedChem 01/2017; 12:33-41., DOI:10.1002/cmdc.201600474
- (A20) Giovanni Macetti, Laura Loconte, Silvia Rizzato, Carlo Gatti, **Leonardo Lo Presti***: *Intermolecular Recognition of the Antimalarial Drug Chloroquine: A Quantum Theory of Atoms in Molecules-Density Functional Theory Investigation of the Hydrated Dihydrogen Phosphate Salt from the 103 K X-ray Structure*. Crystal Growth & Design 09/2016; 16(10):6043-6054., DOI:10.1021/acs.cgd.6b01069
- (A21) Angelo Gavezzotti, Valentina Colombo, **Leonardo Lo Presti***: *Facts and Factors in the Formation and Stability of Binary Crystals*. Crystal Growth & Design 09/2016; 16(10):6095-6104., DOI:10.1021/acs.cgd.6b01146
- (A22) Giulia Rainoldi, Matteo Faltracco, **Leonardo Lo Presti**, Alessandra Silvani*, Giordano Lesma: *Highly diastereoselective entry to chiral spirooxindole-based 4-methyleneazetidines via formal [2+2] annulation reaction*. Chemical Communications 08/2016; 52(77):11575-11578., DOI:10.1039/C6CC05838H (IF: 6.319, Q1(chemistry, multidisciplinary), Cit: 10)
- (A23) Angelo Gavezzotti, **Leonardo Lo Presti***: *Building Blocks of Crystal Engineering: A Large-Database Study of the Intermolecular Approach between C-H Donor Groups and O, N, Cl, or F Acceptors in Organic Crystals*. Crystal Growth & Design 05/2016; 16(5):2952-2962. DOI:10.1021/acs.cgd.6b00305
- (A24) Michael S. Christodoulou*, Mikel Zarate, Francesca Ricci, Giovanna Damia, Stefano Pieraccini, Federico Dapiaggi, Maurizio Sironi, **Leonardo Lo Presti**, Aída Nelly García-Argáez, Lisa Dalla Via*, Daniele Passarella: *4-(1,2-diarylbut-1-en-1-yl)isobutyranilide derivatives as inhibitors of topoisomerase II*. European Journal of Medicinal Chemistry 04/2016; 118:79-89., DOI:10.1016/j.ejmech.2016.03.090
- (A25) Carlo Gatti*, Gabriele Saleh*, **Leonardo Lo Presti**: *Source Function applied to experimental densities reveals subtle electron-delocalization effects and appraises their transferability properties in crystals*. Acta Crystallographica Section B: Structural Science 04/2016; 72(2):180-193., DOI:10.1107/S2052520616003450
- (A26) Giovanni Macetti, Silvia Rizzato, Fabio Beghi, Lucia Silvestrini, **Leonardo Lo Presti***: *On the molecular basis of the activity of the antimalarial drug chloroquine: EXAFS-assisted DFT evidence of a direct Fe-N bond with free heme in solution*. Physica Scripta 02/2016; 91(2-2):023001., DOI:10.1088/0031-8949/91/2/023001

- (A27) Luca Rimoldi, Claudia Ambrosi, Giovanni Di Liberto, **Leonardo Lo Presti***, Michele Ceotto, Cesare Oliva, Daniela Meroni, Serena Cappelli, Giuseppe Cappelletti, Guido Soliveri, Silvia Ardizzone: *Impregnation versus Bulk Synthesis: How the Synthetic Route Affects the Photocatalytic Efficiency of Nb/Ta:N Codoped TiO₂ Nanomaterials*. The Journal of Physical Chemistry C 10/2015; 119(42):24104-24115., DOI:10.1021/acs.jpcc.5b06827
- (A28) Thomas C Eadsforth, Andrea Pinto, Rosaria Luciani, Lucia Tamborini, Gregorio Cullia, Carlo De Micheli, Luciana Marinelli, Sandro Cosconati, Ettore Novellino, **Leonardo Lo Presti**, Anabela Cordeiro-da-Silva, Paola Conti*, William N Hunter*, Maria Paola Costi*: *Characterization of 2,4-Diamino-6-oxo-1,6-dihydropyrimidin-5-yl Ureido Based Inhibitors of Trypanosoma brucei Fold and Testing for Antiparasitic Activity*. Journal of Medicinal Chemistry 08/2015; 58(20):7938-7948., DOI:10.1021/acs.jmedchem.5b00687
- (A29) Angelo Gavezzotti, **Leonardo Lo Presti***: *Theoretical Study of Chiral Carboxylic Acids. Structural and Energetic Aspects of Crystalline and Liquid States*. Crystal Growth & Design 07/2015; 15(8), 3792-3803. DOI:10.1021/acs.cgd.5b00442
- (A30) Lucia Tamborini*, Federica Mastronardi, Federica Dall'Oglio, Carlo De Micheli, Birgitte Nielsen, **Leonardo Lo Presti**, Paola Conti, Andrea Pinto: *Synthesis of unusual isoxazoline containing β and γ -dipeptides as potential glutamate receptor ligands*. MedChemComm 05/2015; 6(7):1260-1266., DOI:10.1039/C5MD00159E
- (A31) Carlo Gatti*, Ahmed Muhammed Orlando, **Leonardo Lo Presti**: *Insights on Spin Polarization through the Spin Density Source Function*. Chemical Science 04/2015; 6(7):3845-3852., DOI:10.1039/C4SC03988B
- (A32) Alessandro Ruffoni*, Alessandro Contini, Raffaella Soave, **Leonardo Lo Presti**, Irene Esposto, Irene Maffucci, Donatella Nava, Sara Pellegrino, Maria Luisa Gelmi, Francesca Clerici*: *Model peptides containing the 3-sulfanyl-norbornene amino acid, a conformationally constrained cysteine analogue effective inducer of 310-helix secondary structures*. RSC Advances 04/2015; 5(41):32643-32656., DOI:10.1039/C5RA03805G
- (A33) Francesca Spadavecchia*, Michele Ceotto, **Leonardo Lo Presti**, Chiara Aieta, Iolanda Biraghi, Daniela Meroni, Silvia Ardizzone, Giuseppe Cappelletti: *Second Generation Nitrogen Doped Titania Nanoparticles: A Comprehensive Electronic and Microstructural Picture*. Chinese Journal of Chemistry 03/2015; 46(9):1195-1213., DOI:10.1002/cjoc.201400502
- (A34) **Leonardo Lo Presti***, Mattia Sist, Laura Loconte, Andrea Pinto, Lucia Tamborini, Carlo Gatti: *Rationalizing the Lacking of Inversion Symmetry in a Noncentrosymmetric Polar Racemate: An Experimental and Theoretical Study*. Crystal Growth & Design 10/2014; 14(11):5822-5833., DOI:10.1021/cg501074x
- (A35) Gabriele Saleh, Carlo Gatti*, **Leonardo Lo Presti***: *Energetics of Non-Covalent Interactions from Electron and Energy Density Distributions*. Computational and Theoretical Chemistry 10/2014; 1053:53-59., DOI:10.1016/j.comptc.2014.10.011
- (A36) Chiara Marchiori, Giovanni Di Liberto, Guido Soliveri, Laura Loconte, **Leonardo Lo Presti***, Daniela Meroni*, Michele Ceotto, Cesare Oliva, Serena Cappelli, Giuseppe Cappelletti, Chiara Aieta, Silvia Ardizzone: *Unraveling the Cooperative Mechanism of Visible-Light Absorption in Bulk N,Nb Codoped TiO₂ Powders of Nanomaterials*. The Journal of Physical Chemistry C 09/2014; 118(41):24152-24164., DOI:10.1021/jp507143z
- (A37) **Leonardo Lo Presti***, Ahmed M. Orlando, Laura Loconte, Riccardo Destro, Emanuele Ortoleva, Raffaella Soave, Carlo Gatti*: *Single N-C Bond Becomes Shorter than a Formally Double N=C Bond in a Thiazete-1,1-dioxide Crystal: An Experimental and Theoretical Study of Strong Crystal Field Effects*. Crystal Growth & Design 08/2014; 14:4418-4429., DOI:10.1021/cg500518a
- (A38) Sara Pellegrino*, Alessandro Contini, Maria Luisa Gelmi, **Leonardo Lo Presti**, Raffaella Soave, Emanuela Erba: *Asymmetric Modular Synthesis of a Semirigid Dipeptide Mimetic by Cascade Cycloaddition/Ring Rearrangement and Borohydride Reduction*. The Journal of Organic Chemistry 03/2014; 79(7):3094-3102., DOI:10.1021/jo500237j
- (A39) **Leonardo Lo Presti***, Michele Ceotto, Francesca Spadavecchia, Giuseppe Cappelletti, Daniela Meroni, Robert G. Acres Silvia Ardizzone: *Role of the Nitrogen Source in Determining Structure and Morphology of N-Doped Nanocrystalline TiO₂*. The Journal of Physical Chemistry C 02/2014; 118(9):4797-4807., DOI:10.1021/jp412394e

- (A40) Mattia Allieta*, Marco Scavini, **Leonardo Lo Presti**, Mauro Coduri, Laura Loconte, Serena Cappelli, Cesare Oliva, Paolo Ghigna, Phil Pattison, Valerio Scagnoli: *Charge ordering transition in GdBaCo₂O₅: Evidence of reentrant behavior*. Physical Review B 12/2013; 88(21):214104., DOI:10.1103/PhysRevB.88.214104
- (A41) Roberta Ettari*, Lucia Tamborini, Ilenia C Angelo, Silvana Grasso, Tanja Schirmeister, **Leonardo Lo Presti**, Carlo De Micheli, Andrea Pinto*, Paola Conti: *Development of Rhodesain Inhibitors with a 3-Bromoisoxazoline Warhead*. ChemMedChem 11/2013; 8(12):2070-2076., DOI:10.1002/cmdc.201300390
- (A42) Gabriele Saleh*, **Leonardo Lo Presti**, Carlo Gatti, Davide Ceresoli: *NClmilano: An electron-density-based code for the study of noncovalent interactions*. Journal of Applied Crystallography 10/2013; 46(5):1513-1517., DOI:10.1107/S0021889813020098
- (A43) Riccardo Destro*, Elisabetta Sartirana, Laura Loconte, Raffaella Soave, Pietro Colombo, Claudio Destro, **Leonardo Lo Presti**: *Competing C=O...C=O, C-H...O, Cl...O, and Cl...Cl Interactions Governing the Structural Phase Transition of 2,6-Dichloro-p-benzoquinone at T_c = 122.6 K*. Crystal Growth & Design 08/2013; 13(10-10):4571-4582., DOI:10.1021/cg401123s
- (A44) Gabriele Saleh, Raffaella Soave*, **Leonardo Lo Presti***, Riccardo Destro: *Progress in the Understanding of the Key Pharmacophoric Features of the Antimalarial Drug Dihydroartemisinin: An Experimental and Theoretical Charge Density Study*. Chemistry - A European Journal 01/2013; 19(10):3490-3503., DOI:10.1002/chem.201202486
- (A45) Gabriele Saleh, Carlo Gatti*, **Leonardo Lo Presti***: *Non-covalent interaction via the reduced density gradient: Independent atom model vs experimental multipolar electron densities*. Computational and Theoretical Chemistry 10/2012; 998:148-163., DOI:10.1016/j.comptc.2012.07.014
- (A46) Francesca Spadavecchia*, Giuseppe Cappelletti, Silvia Ardizzone, Michele Ceotto, Matteo Simone Azzola, **Leonardo Lo Presti**, Giuseppina Cerrato, Luigi Falciola: *Role of Pr on the Semiconductor Properties of Nanotitania. An Experimental and First-Principles Investigation*. The Journal of Physical Chemistry C 10/2012; 116(43):23083-23093., DOI:10.1021/jp307303n
- (A47) Gabriele Saleh, Carlo Gatti*, **Leonardo Lo Presti***, Julia Contreras-García: *Revealing Non-Covalent Interactions in Molecular Crystals through Their Experimental Electron Densities..* Chemistry - A European Journal 10/2012; 18(48):15523-15536., DOI:10.1002/chem.201201290
- (A48) Lucia Tamborini, Andrea Pinto, Terry K Smith, Louise L Major, Maria C Iannuzzi, Sandro Cosconati, Luciana Marinelli, Ettore Novellino, **Leonardo Lo Presti**, Pui E Wong, Michael P Barrett, Carlo De Micheli, Paola Conti*: *Synthesis and Biological Evaluation of CTP Synthetase Inhibitors as Potential Agents for the Treatment of African Trypanosomiasis*. ChemMedChem 08/2012; 7(9):1623-34., DOI:10.1002/cmdc.201200304
- (A49) Tam Luong Nguyen, Maria Rosaria Cera, Andrea Pinto, **Leonardo Lo Presti**, Ernest Hamel, Paola Conti, Rick Gussio, Peter De Wulf*: *Evading Pgp Activity in Drug-Resistant Cancer Cells: A Structural and Functional Study of Antitubulin Furan Metotica Compounds*. Molecular Cancer Therapeutics 03/2012; 11(5):1103-11., DOI:10.1158/1535-7163.MCT-11-1018
- (A50) Michele Ceotto*, **Leonardo Lo Presti***, Giuseppe Cappelletti, Daniela Meroni, Francesca Spadavecchia, Roberto Zecca, Matteo Leoni, Paolo Scardi, Claudia L. Bianchi, Silvia Ardizzone: *About the nitrogen location in nanocrystalline N-doped TiO₂: Combined DFT and EXAFS approach*. The Journal of Physical Chemistry C 01/2012; 116(2):1764-1771., DOI:10.1021/jp2097636
- (A51) **Leonardo Lo Presti***, Mattia Allieta, Marco Scavini, Paolo Ghigna, Laura Loconte, Valerio Scagnoli, Michela Brunelli: *Crystal structure and structural phase transitions in the GdBaCo₂O_{5.0} cobaltite*. Physical review. B, Condensed matter 09/2011; 84(10)., DOI:10.1103/PhysRevB.84.104107
- (A52) **Leonardo Lo Presti***, Arkady Ellern, Riccardo Destro*, Raffaella Soave, Bruno Lunelli: *Rationalizing the Effect of Halogenation on the Molecular Structure of Simple Cyclobutene Derivatives by Topological Real-Space Analysis of Their Electron Density*. The Journal of Physical Chemistry A 07/2011; 115(45):12695-707., DOI:10.1021/jp203615x
- (A53) Emanuele Monza, Carlo Gatti*, **Leonardo Lo Presti***, Emanuele Ortoleva: *Revealing Electron Delocalization through the Source Function*. The Journal of Physical Chemistry A 07/2011; 115(45):12864-78., DOI:10.1021/jp204000d

- (A54) Lucia Tamborini*, Andrea Pinto, Paola Conti, Maddalena Gallanti, MC Iannuzzi, **Leonardo Lo Presti**, Carlo De Micheli: *Regioselective Preparation of Functionalized Isoxazoline Derivatives as Key Intermediates for the Synthesis of Selective N-Methyl-D-aspartate Receptor Antagonists*. Synthesis 04/2011; , DOI:10.1055/s-0030-1258477
- (A55) Luca Beverina*, Alessandro Sanguineti, Glauco Battagliarin, Riccardo Ruffo, Dominique Roberto, Stefania Righetto, Raffaella Soave, **Leonardo Lo Presti**, Renato Ugo, Giorgio A Pagani*: *UV absorbing zwitterionic pyridinium-tetrazolate: Exceptional transparency/optical nonlinearity trade-off*. Chemical Communications 01/2011; 47(1):292-4., DOI:10.1039/c0cc01652g
- (A56) **Leonardo Lo Presti***, Raffaella Soave, Mariangela Longhi, Emanuele Ortoleva: *Conformational polymorphism in a Schiff-base macrocyclic organic ligand: An experimental and theoretical study*. Acta crystallographica. Section B, Structural science 10/2010; 66(Pt 5):527-43., DOI:10.1107/S0108768110029514
- (A57) Clelia Dallanoce*, Pietro Magrone, Carlo Matera, **Leonardo Lo Presti**, Marco De Amici, Loredana Riganti, Francesco Clementi, Cecilia Gotti, Carlo De Micheli: *Synthesis of novel chiral Δ^2 -isoxazoline derivatives related to ABT-418 and estimation of their affinity at neuronal nicotinic acetylcholine receptor subtypes*. European Journal of Medicinal Chemistry 09/2010; 45(12):5594-601., DOI:10.1016/j.ejmech.2010.09.009
- (A58) Ahmed M Orlando, **Leonardo Lo Presti***, Raffaella Soave: *A new monoclinic polymorph of 3-diethyl-amino-4-(4-methoxy-phenyl)-1,1-dioxo-4H-1 λ ,2-thia-zete-4-carbonitrile*. Acta Crystallographica Section E Structure Reports Online 08/2010; 66(Pt 8):o2032-3., DOI:10.1107/S1600536810027558
- (A59) Riccardo Destro*, Emanuele Ortoleva, Raffaella Soave, Laura Loconte, **Leonardo Lo Presti**: *Detection and kinetics of the single-crystal to single-crystal complete transformation of a thiranium ion into thietanium ion*. Physical Chemistry Chemical Physics 10/2009; 11(33):7181-8., DOI:10.1039/b901928f
- (A60) **Leonardo Lo Presti***, Carlo Gatti*: *Using the Source Function descriptor to dampen the multipole model bias in charge density studies from X-ray structure factors refinements*. Chemical Physics Letters 07/2009; 476(4-6):308-316., DOI:10.1016/j.cplett.2009.06.022
- (A61) **Leonardo Lo Presti***, Arkady Ellern, Riccardo Destro, Bruno Lunelli: *Effect of Methoxy Substituents on the Structural and Electronic Properties of Fluorinated Cyclobutenes: A Study of Hexafluorocyclobutene and Its Vinyl Methoxy Derivatives by XRD and Periodic DFT Calculations*. The Journal of Physical Chemistry A 05/2009; 113(13):3186-96., DOI:10.1021/jp8084809
- (A62) **Leonardo Lo Presti***, Riccardo Destro: *Experimental and theoretical charge density distribution of the colossal magnetoresistive transition metal sulfide FeCr₂S₄*. The Journal of Chemical Physics 02/2008; 128(4):044710., DOI:10.1063/1.2822160
- (A63) **Leonardo Lo Presti***, Raffaella Soave, Riccardo Destro: *On the Interplay between CH...O and OH...O Interactions in Determining Crystal Packing and Molecular Conformation: An Experimental and Theoretical Charge Density Study of the Fungal Secondary Metabolite Austdiol (C₁₂H₁₂O₅)*. The Journal of Physical Chemistry B 04/2006; 110(12):6405-14., DOI:10.1021/jp056823y
- (A64) **Leonardo Lo Presti**, Donatella Invernizzi, Raffaella Soave, Riccardo Destro*: *Looking for structural phase transitions in the colossal magnetoresistive thiospinel FeCr₂S₄ by a multi-temperature single-crystal X-ray diffraction study*. Chemical Physics Letters 11/2005; 416(1-3):28-32., DOI:10.1016/j.cplett.2005.09.037
- (A65) Riccardo Destro*, Raffaella Soave, Mario Barzaghi, **Leonardo Lo Presti**: *Progress in the Understanding of Drug-Receptor Interactions, Part 1: Experimental Charge-Density Study of an Angiotensin II Receptor Antagonist (C₃₀H₃₀N₆O₃S) at T=17 K*. Chemistry-A european Journal 08/2005; 11(16):4621-34., DOI:10.1002/chem.200400964
- (A66) Riccardo Destro*, Laura Loconte, **Leonardo Lo Presti**, Pietro Roversi, Raffaella Soave: *On the role of data quality in experimental charge-density studies*. Acta Crystallographica Section A Foundations of Crystallography 10/2004; 60(Pt 5):365-70., DOI:10.1107/S0108767304014813
- (A67) **Leonardo Lo Presti**, Raffaella Soave*, Riccardo Destro: *The Fungal Metabolite Austdiol (I)*. Acta Crystallographica Section C Crystal Structure Communications 08/2003; 59(Pt 4):O199-201., DOI:10.1002/chin.200334211

(A68) Francesca Clerici*, Maria Luisa Gelmi, Raffaella Soave, **Leonardo Lo Presti**: *Isothiazoles. Part 13. Synthesis of Sulfamic Esters, [1,2]Thiazete S,S-Dioxides, Benzo[e][1,2]thiazine S,S-Dioxides or Triazoles by Reaction of Isothiazole Dioxides with Sodium Azide*. Tetrahedron 06/2002; 58(25):5173-5178., DOI:10.1016/S0040-4020(02)00445-3

Book Chapters

- C. Gatti, A. M. Orlando, E. Monza, **L. Lo Presti**, “Exploring Chemistry Through the Source Function for the Electron and the Electron Spin Densities”, invited monography for the book on “Applications of Topological Methods in Molecular Chemistry”, Ed. R. Chauvin, C. Lepetit, B. Silvi, E. Alikhani, on behalf of Springer Ed. (2016), DOI: 10.1007/978-3-319-29022-5_5; ISBN: 978-3-319-29020-1. Cit: 0 (Altmetry: 611 downloads)
- R. Destro, R., **L. Lo Presti**, R. Soave, A. E. Goeta, “Multi-temperature charge density studies”, invited monography for the book on “Modern Charge Density Analysis”, Ed. C. Gatti and P. Macchi, on behalf of Springer Ed. (2010), DOI: 10.1007/978-90-481-3836-4_19; ISBN: 978-90-481-3835-7. Cit: 2 (Altmetry: 1.15 k downloads)

Oral Presentations (presenting person underlined).

(O1) **A crystallographic route to understand drug solubility: the case of 4-aminoquinoline antimalarials**
Leonardo Lo Presti, Silvia Rizzato

Invited keynote lecture at the international MISCA-V conference (Meeting of the Italian and Spanish Crystallographic Associations), Naples, Italy, September 4-7, 2019 ([forthcoming](#))

(O2) **Structural and electronic properties of N-doped TiO₂/SnO₂ photocatalysts for air pollutant remediation**

Daniela Meroni, Laura Tripaldi, Luca Rimoldi, **Leonardo Lo Presti**

Co-author in a contributed talk at the International Symposium on Inorganic and Environmental Materials (ISIEM2018), Pand - Onderbergen, Ghent, Belgium, June 17-21, 2018.

(O3) **Gaining insights on chemistry from the analysis of the charge density**

Leonardo Lo Presti

Invited talk at the CrisDi workshop on “The Role of Crystallography in Drug Science and Biology”, Torino, Italy, 05 March 2018

(O4) **On the interplay among non-covalent interactions and activity of 4-Aminoquinoline antimalarials: A crystallographic and spectroscopic study**

Leonardo Lo Presti, Silvia Rizzato, Pietro Sacchi, Giovanni Macetti, Laura Loconte, Fabio Beghi, Lucia Silvestrini

Presenting Author in a contributed talk at the XLVI Annual Meeting of the Italian Crystallographic Association, Perugia, Italy, 26 - 29 June 2017

(O5) **Silver nanoparticles/nanostructured TiO₂ interface: a photo -renewable “silver-ions electrode” for neurotransmitters detection**

Valentina Pifferi, Giovanni Di Liberto, Guido Soliveri, Guido Panzarasa, Daniela Meroni, Silvia Ardizzone, Michele Ceotto, **Leonardo Lo Presti**, Luigi Falciola

Co-Author in a contributed talk at the XXI Topical Meeting of the International Society of Electrochemistry, Szeged, Hungary, 23 - 26 April 2017

(O6) **Study of the key interactions in the self-recognition of an antimalarial drug**

Giovanni Macetti, Silvia Rizzato, Laura Loconte, Carlo Gatti, **Leonardo Lo Presti**

Co-Author in a contributed talk at the 7th European Charge Density Meeting (ECDM-7), Warsaw, Poland, 16 June - 1 July 2016

(O7) **Photo-renewable electroanalytical sensor for neurotransmitter detection: the role of silver ion nanoparticles**

Valentina Pifferi, Giovanni Di Liberto, Guido Soliveri, Guido Panzarasa, Michele Ceotto, **Leonardo Lo Presti**, Luigi Falciola

Co-Author in a contributed plenary lecture at the 16th International Conference on Electroanalysis (ESEAC 2016), The Assembly Rooms, Bath, June 12-16, 2016

(O8) **Silver cations electroanalytical sensor: sensitivity and selectivity in the detection of neurotransmitters**

Valentina Pifferi, Giovanni Di Liberto, Guido Soliveri, Guido Panzarasa, Michele Ceotto, **Leonardo Lo Presti**, Luigi Falciola

Co-Author in a contributed talk at the 3rd Sensor National Congress (Convegno Nazionale Sensori), CNR hall, Piazzale Aldo Moro 7, Rome, Italy, February 23-25, 2016

(O9) **Principal component analysis methods applied to crystallographic and charge density problems**

Leonardo Lo Presti, Angelo Gavezzotti

Contributed talk at the Centre for Materials Crystallography (CMC) annual meeting, Goettingen, Germany, 28-30 January, 2016

(O10) **Synchrotron radiation in environmental remediation: Shedding light on the structural and electronic properties of second generation photocatalysts**

Daniela Meroni, **Leonardo Lo Presti**, Michele Ceotto, Giuseppe Cappelletti

Co-Author in a keynote lecture at the XXIII SILS (Società Italiana di Luce di Sincrotrone) Meeting, via Tommaso Gar 14, Trento, Italy, July 8-10, 2015

(O11) **Unveiling interactions of the antimalarial drug chloroquine with haeme in aqueous solutions through spectroscopic and quantum mechanical methods**

Leonardo Lo Presti, Giovanni Macetti, Fabio Beghi, Silvia Rizzato

Contributed talk at the at the SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities, Santa Margherita di Pula (CA), Italy, June 7-12, 2015

(O12) **Progettazione di nuovi materiali per l'abbattimento di inquinanti : Come proteggere i nostri monumenti (Development of novel materials for pollutant remediation: How to protect our cultural heritage)**

Michele Ceotto, Giuseppe Cappelletti, Dario Tamascelli, Paola Fermo, Luigi Falciola, **Leonardo Lo Presti**, Silvia Ardizzone

Co-Author in a contributed talk at the National Meeting on "High-performance computing for innovation and competitiveness of research and small-medium enterprises in Lombardy: Calls for the LISA 2014 initiative and opportunities for the H2020 program" ("Il calcolo ad alte prestazioni per l'innovazione e la competitività della ricerca e delle PMI lombarde : I bandi LISA 2014 e le opportunità nell'ambito di Horizon 2020"), Grattacielo Pirelli, Milano (Italy), February 18, 2014

(O13) **Understanding the lacking of inversion symmetry in an acentric polar racemate**

Leonardo Lo Presti, Mattia Sist, Laura Loconte, Carlo Gatti

Contributed talk at the Centre for Materials Crystallography (CMC) annual meeting, Aarhus, Denmark, October 8-10, 2014

(O14) **Doped nano-titania: theoretical insight into structure-property relationships**

Michele Ceotto, **Leonardo Lo Presti**, Laura Loconte, Daniela Meroni, Luigi Falciola, Valentina Pifferi, Guido Soliveri, Giuseppe Cappelletti, Chiara D. Aieta, Robert G. Acres, Silvia Ardizzone

Co-Author in a contributed talk at XXV National Congress of the Italian Chemical Society (Congresso Nazionale della Società Chimica Italiana, SCI-2014), Arcavacata di Rende, Italy, September, 7-12 2014

(O15) **Doped Titania Nanocrystals Explained By Experimental And DFT Characterizations**

Michele Ceotto, **Leonardo Lo Presti**, Giuseppe Cappelletti, Luigi Falciola, Daniela Meroni, Francesca Spadavecchia, Silvia Ardizzone

Co-Author in a contributed talk at XL National Congress of Physical Chemistry, Alessandria, Italy June 23-27, 2013

(O16) **Revealing electron delocalization through the Source Function**

Carlo Gatti, Emanuele Monza, **Leonardo Lo Presti**, Gabriele Saleh

Co-Author in a contributed talk at the 1st National Congress of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society, Pisa, February 22-23, 2012

(O17) **Using X-ray Derived Charge Densities to Detect Electron Delocalization Effects and Non-covalent Interactions**

Carlo Gatti, Gabriele Saleh, **Leonardo Lo Presti**

Co-Author in an invited talk at the 6th European Charge Density Meeting (ECDM-6), Štrbské pleso, Slovakia, September 15-20, 2012

(O18) **Making experiments and theory talking together: electron delocalization effects and non-covalent interactions detection via the Source Function and the Reduced Density Gradient**

Carlo Gatti, Gabriele Saleh, *Leonardo Lo Presti*, Emanuele Monza
Co-Author in an invited talk at the SAGAMORE XVII Conference on Charge, Spin and Momentum Densities: “Great potentials for Advances Probes”, Daini Mesui Tei, Hokkaido, Japan, 15-20 July 2012

(O19) Revealing electron delocalization through the Source Function

Carlo Gatti, Emanuele Monza, *Leonardo Lo Presti*, Gabriele Saleh
Co-Author in a invited talk at the symposium “X-ray and Neutron Scattering for Solving Structures and Modelling Charge Densities: The Last 40 Years (A colloquium in honor of Pierre J. Becker)”, Chateau des sept tours 37330, Courcelles de Touraine, France, September 16-17, 2011

(O20) Evaluation of the Source Function in C₄F₆ and Mn₂(CO)₁₀

Carlo Gatti, *Leonardo Lo Presti*
Invited practical tutorial (30’) at the Workshop on XD2006 Program Package “Advanced Methods in X-ray Charge Density Analysis: Extracting Properties from a Multipole Refinement”, Martina Franca, Italy, 3-6 September, 2007

(O21) Exploring a phase transition by a charge-density study

Elisabetta Sartirana, Laura Loconte, *Leonardo Lo Presti*, Raffaella Soave, Riccardo Destro
Co-Author in a contributed talk at the 4th European Charge Density Meeting (ECDM-IV), Brandenburg on the Havel, Germany, January 26-29, 2006

(O22) Gain from charge-density-quality X-ray diffraction experiment

Riccardo Destro, Laura Loconte, *Leonardo Lo Presti*, Raffaella Soave
Co-Author in a contributed talk at the 3rd European Charge Density Meeting (ECDM-3), Sandbjerg Estate, Denmark, June 24-29, 2003

Posters (presenting person underlined)

(P1) Correlations among solubility and crystal structure: a crystallographic and spectroscopic study of the antimalarial drug piperazine

Pietro Sacchi, Giovanni Macetti, Silvia Rizzato, Laura Loconte, Fabio Beghi, *Leonardo Lo Presti*
Co-author in poster session at the 3rd joint AIC-SILS conference, Rome, Italy, 25-28 June 2018

(P2) Correlations among solubility and crystal structure: a crystallographic and spectroscopic study of the antimalarial drug piperazine (precedente versione, con risultati preliminari, del poster P1)

Pietro Sacchi, Giovanni Macetti, Silvia Rizzato, Laura Loconte, Fabio Beghi, *Leonardo Lo Presti*
Co-author in poster session at the congress Italian Crystal Growth 2017, Milano, Italy, 20-21 November 2017

(P3) Synthesis and evaluation of bicyclo[3.1.0]hexane carboxylic acids as candidate inhibitors of influenza A neuraminidases

Cinzia Colombo, C. Podlipnik, *Leonardo Lo Presti*, Anna Bernardi, B. M. Pinto, A. J. Bennet
Co-author in poster session at the Carbohydrates Gordon Research Conference, Mount Snow West Dover, VT, USA, 25 - 30 June 2017

(P4) Nanoparticles Based on Fructose and Alkali-Earth Halogenides with Second Harmonic Generation properties for applications as bio-sensors and for Radiotherapy

Domenica Marabello, Paola Antoniotti, Alessandro Barge, Paola Benzi, Valentina Boscaro, Carlo Canepa, Margherita Gallicchio, Elena Peira, *Leonardo Lo Presti*
Co-Author in poster session at the the XLVI Annual Meeting of the Italian Crystallographic Association, Perugia, Italy, 26 - 29 June 2017

(P5) Source Function applied to experimental densities reveals subtle electron delocalization effects and appraises their transferability properties in crystals

Carlo Gatti, Gabriele Saleh, *Leonardo Lo Presti*
Co-Author in poster session at the 7th European Charge Density Meeting, Warsaw, Poland, June 26-July 1, 2016

(P6) Experimental and theoretical study of the mechanism of action of the antimalarial drug chloroquine

Giovanni Macetti, Silvia Rizzato, Laura Loconte, Carlo Gatti, *Leonardo Lo Presti*
Co-Author in poster session at the 4th meeting of the Italian and Spanish Crystallographic Associations (MISCA-4), Puerto de la Cruz, Tenerife, Spain, June 21-25, 2016

(P7) **Non-innocent role of ligands in some Ni organometallic complexes as viewed through the spin density source function**

Ahmed. M. Orlando, Carlo Gatti, *Leonardo Lo Presti*

Co-Author in poster session at the XXIX European Crystallographic Meeting, Rovinj, Croatia, August 23-28, 2015

(P8) **Looking for indirect correlations among charge density and NLO properties: the case of a simple pyridinium tetrazolate**

Authors: Fabio Beghi, Emanuele Ortoleva Raffaella Soave, Laura Loconte, *Leonardo Lo Presti*

Co-Author in poster session at the SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities, Santa Margherita di Pula (CA), Italy, June 7-12, 2015

(P9) **Understanding self-recognition in the antimalarial drug chloroquine: an experimental and theoretical charge density study**

Giovanni Macetti, Silvia Rizzato, Laura Loconte, Carlo Gatti, *Leonardo Lo Presti*

Co-Author in poster session at the SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities, Santa Margherita di Pula (CA), Italy, June 7-12, 2015

(P10) **Decoding conformational polymorphism in a thiazete-1,1-dioxide**

Authors: Ahmed M. Orlando, Laura Loconte, Carlo Gatti, *Leonardo Lo Presti*

Co-Author in poster session at the SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities, Santa Margherita di Pula (CA), Italy, June 7-12, 2015

(P11) **Towards the understanding of structure-properties relationships in N,Nb doped TiO₂ nanopowders: a multidisciplinary experimental and DFT approach**

Leonardo Lo Presti, Michele Ceotto, Daniela Meroni, Francesca Spadavecchia, Laura Loconte, Luigi Falciola, Giuseppe Cappelletti, Silvia Ardizzone

Presented at the SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities, Santa Margherita di Pula (CA), Italy, June 7-12, 2015

(P12) **Second generation photocatalysts by metal and nitrogen codoping. The role of Ta and Nb**

Luca Rimoldi, Claudia Ambrosi, Guido Soliveri, Giuseppe Cappelletti, Serena Cappelli, Michele Ceotto, *Leonardo Lo Presti*, Daniela Meroni, Cesare Oliva, Silvia Ardizzone

Co-Author in poster session at the Fifth International Conference on Semiconductor Photochemistry (SP5), Saint Petersburg, Russian Federation, July 27-31, 2015

(P13) **Decoding conformational polymorphism in organic substances**

Ahmed M. Orlando, Laura Loconte, Emanuele Ortoleva, Carlo Gatti, *Leonardo Lo Presti*

Co-Author in poster session at the XXIII International Union of Crystallography Congress, Montreal, Canada, August 5-12, 2014

(P14) **Conformational polymorphism in a thiazete-1,1 dioxide derivative: a charge density study**

Ahmed M. Orlando, *Leonardo Lo Presti*, Laura Loconte, Emanuele Ortoleva

Co-Author in poster session at the workshop "Natta's Seeds Grow: From the crystallography and modeling of stereoregular polymers to the challenges of complex systems", Politecnico di Milano, Milano, Italy, November 21-22, 2013

(P15) **Chemical bonding and intermolecular interactions of a non-centrosymmetric racemate with Z'=2**

Mattia Sist, *Leonardo Lo Presti*, Laura Loconte, Carlo Gatti

Co-Author in poster session at the workshop "Natta's Seeds Grow: From the crystallography and modeling of stereoregular polymers to the challenges of complex systems", Politecnico di Milano, Milano, Italy, November 21-22, 2013

(P16) **Experimental and theoretical charge density study of an antimalarial drug**

Raffaella Soave, Gabriele Saleh, *Leonardo Lo Presti*, Riccardo Destro

Co-Author in poster session at the workshop "Natta's Seeds Grow: From the crystallography and modeling of stereoregular polymers to the challenges of complex systems", Politecnico di Milano, Milano, Italy, November 21-22, 2013

(P17) **NCImilano: an Electron Density based code for the study of Non-Covalent Interactions**

Gabriele Saleh, Carlo Gatti, *Leonardo Lo Presti*

Co-Author in poster session at the Gordon 2013 Research Conference on Electron Distribution & Chemical Bonding: Pushing the Limits of Experimental and Theoretical Charge and Spin Density Studies, Les Diablerets, Switzerland, June 02-07, 2013

(P18) **Non-covalent interactions descriptor using experimental electron densities**

Gabriele Saleh, Carlo Gatti, *Leonardo Lo Presti*, Julia Contreras-Garcia

Co-Author in poster session at the "Small Molecules in Interactions, International Symposium", Faculty of Chemistry Ruhr Universität Bochum, Germany (DK), March 26-27, 2012

(P19) Non-Covalent Interactions Revealed by Mapping the Energy Density on the Reduced Density Gradient Isosurfaces

Gabriele Saleh, Carlo Gatti, *Leonardo Lo Presti*

Co-Author in poster session at the VI European Charge Density Meeting ECDM-6, Štrbské Pleso, Slovakia, September 15-20, 2012

(P20) Revealing electron conjugation through an observable

Carlo Gatti, Emanueele Monza, *Leonardo Lo Presti*, Gabriele Saleh

Co-Author in poster session at the XXII IUCr Congress, Madrid, Spain, August 22-30, 2011

(P21) Non-Covalent Interactions descriptor using experimental electron densities

Gabriele Saleh, Carlo Gatti, *Leonardo Lo Presti*, Julia Contreras-Garcia

Co-Author in poster session at the XXII IUCr Congress, Madrid, Spain, August 22-30, 2011

(P22) Using the Source Function to reveal and dampen the Multipole Model bias in Charge Density Studies from X-ray structure factors refinements

Carlo Gatti, *Leonardo Lo Presti*

Co-Author in a poster session at the SAGAMORE XVI Conference on Charge, Spin and Momentum Densities, Santa Fe, New Mexico (USA), 2-7 August, 2009

(P23) The Multipolar Model Bias on Primary Densities as revealed by the source Function Descriptor

Leonardo Lo Presti, Carlo Gatti

Presented at the 5th European Charge Density Meeting, Gravedona, Lake Como, Italy, June 6-11, 2008

(P24) The phase transition of chloranil: an experimental and theoretical study

Leonardo Lo Presti, Elisabetta Sartirana, Laura Loconte, Raffaella Soave, Riccardo Destro

Presented at the School of Ab-Initio Modeling in Solid State Chemistry (MSSC-2006), University of Torino, Turin, Italy, September 03-09, 2006

Conference papers

(C1) Insights on spin-density delocalization/polarization mechanisms through the source function

Carlo Gatti, G. Macetti, L. Lo Presti, Acta Crystallographica Section A 2017, 73(a2):C1434-C1434, DOI: 10.1107/S2053273317081426

(C2) Non-innocent role of ligands in some Ni organometallic complexes as viewed through the spin density source function

A. M. Orlando, C. Gatti, L. Lo Presti, Acta Crystallographica Section A 2015, 71(a1):s416-s416, DOI: 10.1107/S2053273315093857

(C3) Decoding conformational polymorphism in organic substances

A. M. Orlando, L. Loconte, E. Ortoleva, C. Gatti, L. Lo Presti, Acta Crystallographica Section A 2014, 70(a1):C557-C557, DOI: 10.1107/S205327331409442X

(C4) Non-Covalent Interactions descriptor using experimental electron densities

G. Saleh, C. Gatti, L. Lo Presti, J. Contreras-García, Acta Crystallographica Section A 2011, 67(a1) C448, DOI: 10.1107/S0108767311088702

(C5) Revealing electron conjugation through an observable

C. Gatti, E. Monza, L. Lo Presti, G. Saleh, Acta Crystallographica Section A 2011, 67(a1) C443, DOI: 10.1107/S0108767311088829
