Leonardo Lo Presti, Ph.D.

Associate Professor of Physical Chemistry (CHIM/02, Chimica Fisica) at Università degli Studi di Milano

General Indicators

Reseracher 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
Website: https://sites.unimi.it/xtal_chem_group/

Publications in the last 5 years (2019–2024): **40**
Total number of papers (2002-2024): **106**
Book chapters: **3**

H-index (total, WoS): 24
H-index (total, Scopus): 24
H-index (total, Google Scholar): 26

i-10-index (Google Scholar): 70

Total citations (WoS): 2024
Total citations (Scopus): 2116
Total citations (Google Scholar): 2511

Career

Graduated in Chemistry at the University of Milan with honors in 2000, I embarked on the PhD course in Chemical Sciences (XVI cycle, 2000-2003). After the post-doc (2003-2007), in 2007 I won a position as Researcher (RU) at the University of Milan and subsequently as Associate Professor (2019) in the scientific-disciplinary sector CHIM/02.

Short Overview

I am a **chemical crystallographer**. My interests are in **materials science**, with particular focus on **molecular recognition** and **structure-property relationships**. I develop predictive theories of the solid state for organic molecular crystals, trying to understand crystal nucleation at the molecular level. The aim is to discover the general laws that correlate the molecular physicochemical properties to the actually observable crystalline structures. I am the main author of the **MiCMoS software** for the simulation of small organic molecules in the condensed phase using classical Monte Carlo and Molecular Dynamics techniques. The program can be downloaded for free at: https://sites.unimi.it/xtal_chem_group/index.php/research/5-micmos.

Concerning hard materials, I study the structure/property relationships of transition metal oxides at various size scales with synchrotron light (X-ray powder diffraction, X-ray absorption spectroscopy) and computational methods (periodic quantum simulations).

Detailed Overview

Since 2011, I lead the XtalChem Group @ Università degli studi di Milano. My first expertise is in highresolution single-crystal X-ray diffraction and real-space analysis of the charge density distribution. Over the years, I also acquired skills on quantum mechanical simulations in the solid state, X-ray powder diffraction and EXAFS spectroscopy. Now, we do research on solid-state and

condensed-state cutting edge problems, such as structure-activity correlations in complex materials (TiO_2-based photocstalysts, methylammonium bromide lead perovskites and transition metal perovskites) and aggregation phenomena in small organic molecules.

Until 2020, I coordinated the work of a graduate technician (Laura Loconte, laura.loconte@unimi.it), who is a physicist expert in instrumentation for single-crystal X-ray diffraction. I was the tutor of 6 PhD students (L. Sironi, cycle XXXIX, G. Bruno, cycle XXXIV, F. Menescardi, cycle XXXIII, G. Macetti, cycle XXXI; A. M. Orlando, cycle XXVIII; G. Saleh, cycle XXVI), while I became the tutor of another one (S. Cenedese, cycle XXIV) only after prof. Destro's retirement. Fellowships of Macetti, Orlando and Saleh were entirely funded by the Centre of Materials Crystallography (CMC) at Århus in Denmark, to which I used to be associated (see International Collaborations). In the period 2011-2024 I was also the tutor of 19 MSc students (M. Vacchini, M. Brocca, L. Sironi, F. Marinoni, G. Finocchio, G. Tusha, M. Frigerio, A. Sala, D. Rosa, P. Sacchi, A. Gionda, G. Buccella, G. Bruno, F. Beghi, G. Macetti, C. Tantardini, M. Sist, V. Pugliese, A. M. Orlando), 14 BSc students (A. G. Valsecchi, A. Cambiaghi, F. Golini, L. Ginelli, M. Vacchini, D. Mondonico, L. Tana, A. Pisati, L. Invernizzi, L. Chiesa, F. Marinoni, P. Zaglio, M. Frigerio e M. Draghetti), and co-tutor of several MSc and BSc students.

My group exploits collaborations with various scientists in both Italy and Europe, testified by co-authorships in recent published works. Of particular relevance are collaborations with permanent staff at the INFN (Dr. Marianna Testa), La Sapienza (prof. Eugenio Delr Re), Institute of Molecular Science and Technology (ISTM) of the Italian CNR (Carlo Gatti, Aminoff laureate - retired - and Dr. Raffaella Soave), with the molecular biologist Dr. Lucia Silvestrini at University of Natural Resources and Life Sciences (now working at Università vita-salute San Raffaele, Milan) and with various beamline scientists worldwide (among others, Dr. Robert G. Acres, currently at the Australian Synchrotron in Notting Hill, and Dr. Kevin Prince, at ELETTRA (Trieste, Italy)). I also collaborate with various groups at the Department of Chemistry and at the Department of Pharmaceutical Sciences at Università degli Studi di Milano, to which I provide assistance in determining the chemical structure of novel synthesis products by single crystal X-ray diffraction methods.

Among my reserch interests, the study of nucleation has great relevance. The final goal is to gain isights on the molecular mechanism(s) underlying self-recognition in organic molecular crystals and to develop a predictive theory of crystallization - a sort of Holy Grail of crystallography. To reach this goal, I employ experimental methods to study aggregation in solution (XAS techniques) and to investigate the crystal structure (single-crystal X-ray diffraction), and computational techniques, including data-mining on large databases. I am the main author of the Milano Chemistry Molecular Simulation (MiCMoS) software, intended to perform Monte Carlo and Molecular Dynamics simulations of small organic molecules in condensed phases, including liquids, solutions and crystalline or amorphous solids. The software is freely available from the web page of my group (https://sites.unimi.it/xtal_chem_group/index.php/research/5-micmos) and was downloaded and employed by more than 60 groups worldwide by now.

Funding

I won a total of 20 national and international competitive grants to obtain machine time at synchrotron / neutron light sources and high performance computational resources (CINECA calls: 4 ISCRA-C, 3 LISA). All the proposed projects were evaluated by anonymous experts according to the practices of peer review.

I am currently the coordinator of a local unit of the PRIN2022 project "Harnessing ferroelectric topological defects for photonics (FERROKNOTS)" led by prof. Eugenio del Re (La Sapienza). My funding amounts to 58647,00 €.

I won 1 local SEED "Seal of Excellence" grant (2021-2022) of 30000 € (project: GO-LIFE).

In 2018 I won a grant from the MIUR's Annual Financing Fund for Basic Research Activities (FFABR) for the competitive selection of the quality of scientific publications (3000 €).

I was entitled of 2 local grants under the "University Development Plan" of the University of Milan

for the enhancement of scientific excellence: 2014-2015: UNIAGI 17777, 6800 €; 2016-2017: NOVAQ, 9250 €.

In 2009, I participated in a PUR 2008 financed project (2009-ATE-0119, funding: 12000 €), whose PI was prof. Riccardo Destro.

PARTICIPATION AS A STAFF MEMBER IN EU-FUNDED PROJECTS I participated as a scientific staff member to the ERC consolidator project SEMICOMPLEX (PI: prof. Michele Ceotto, see https://cordis.europa.eu/project/id/647107), financed by the European Union. I was entrusted as an expert in solid state chemistry and crystallography to investigate surfaces and solid-solid interfaces from a computational point of view.

Technology Transfer

Patent holder (13%, number 102023000012477) for a high-energy particle sensor based on methylammonium halogenide perovskite single crystals. The patent is now being evaluated for approvation.

Awards

As a student, 100% exemption of university fees for curricular merits.

Recipient of a PhD scholarship to the school in Chemistry (2000–2003).

Winner of a two-year research grant, then renewed once, at the Department of Physical Chemistry and Electrochemistry of the University of Milan (2003–2007).

National Award of the Italian Crystallography Association (AIC) for the best crystallographic thesis: awarded in 2015 to an experimental thesis entitled "Experimental and Theoretical Study of the Mechanism of Action of the Antimalarial Drug Chloroquine" presented by my master student John Macetti. This thesis work has produced two scientific publications (DOI: 10.1088/0031-8949/91/2/023001; DOI: 10.1021/acs.cgd.6b01069).

National Award of the Italian Crystallography Association (AIC) for the best crystallographic thesis: awarded in 2018 to an experimental thesis entitled "Correlations among solubility and crystal structure: a crystallographic and spectroscopic study of the antimalarial drug piperaquine" presented by my master student Pietro Sacchi. This thesis work has produced a scientific publication (DOI: 10.1021/acs.cgd.8b01794).

National Award of the Italian Crystallography Association (AIC) for the best crystallographic master thesis: awarded in 2022 to an experimental thesis entitled "Combined Experimental and Computational Studies on Molecular Recognition among D-Glucose Molecules" presented by my master student Luca Sironi. This thesis work has produced a scientific publication (DOI: 10.1021/acs.cgd.2c00846).

I obtained the National Scientific Habilitation for the functions of second level Professor (**Professore Associato**) for the Scientific-Disciplinary Sectors **03/A2** (MODELS AND METHODOLOGIES FOR CHEMICAL SCIENCES, from 10/04/2017 to 10/04/2028) and **03/B1** (FOUNDATIONS OF CHEMICAL SCIENCES AND INORGANIC SYSTEMS, from 12/04/2017 to 12/04/2028). I also obtained the National Scientific Habilitation for the functions of full Professor **(Professore Ordinario**) for the SSD **03/A2** (from 05/06/2023 to 05/06/2034) and for the SSD **03/B1** (from 06/12/2023 to 06/12/2034).

National Collaborations

From 01/01/2021 to 31/12/2023 I have a partnerhip with the **Istituto Nazionale di Fisica Nucleare - Laboratori Nazionali di Frascati** (INFN-LNF) within an INFN- funded grant for the development for advanced perovskite sensors for high-energy applications. In particular, I deal with the experimental investigation by means of X-ray diffraction techinques of methyhalamonium bromide lead perovskites to study the structure of the material at different

length scales. The idea is to correlate the structural information with voltage-current responses measured at Frascati, to gain insights into solid-state transport phenomena and increase the amplification performance of the device.

Since July, 22 2017 and until July, 22 2019, I had a partnership with the **Institute of Molecular Sciences and Technologies** (Istituto di Scienze e Tecnologie Molecolari, ISTM) **of the Italian CNR**. Project DCM.AD002.122 / CMC CENTER OF MATERIALS CRYSTALLOGRAPHY Title: Experimental and theoretical study of bulk correlated materials with potential chemical and tecnological interest. The project was devoted to correlated materials. I studed ferroelectric relaxors with perovskite structure exhibiting exceptional optical properties, such as index of refraction >30, which can be used to produce innovative optical devices with no chromatic aberration. Moreover, I also performed solid-state computational studies of non-linear optical (NLO) metal-organic frameworks based on beta-D fructopyranose and alkaline earth halides.

In 2011-2014 I had a partnership with the **Institute of Molecular Sciences and Technologies** (Istituto di Scienze e Tecnologie Molecolari, ISTM) **of the Italian CNR**. I was involved in a project of the Department of Chemical Sciences and Materials Technologies with the following specs: Project PM.P07 (Predictive functional modelling of nanostructured systems of biological and nanotechnological interest; Modelling predittivo delle funzionalità in sistemi nanostrutturati di interesse biologico e tecnologico); Commission PM.07.002 (Computational and structural chemical nanoengineering; Nanoingegneria chimica computazionale e strutturale); Module PM.07.002.001 (Experimental and theoretical chemical nanoengineering: analysis of the electron density distributions through innovative computational methods and high-resolution X-ray diffraction techniques; Nanoingegneria chimica sperimentale e teorica: analisi di distribuzioni di densità elettronica con metodi computazionali innovativi e tecniche di diffrazione di raggi X ad alta risoluzione). The CNR permanent staff member responsible for this research line is Dr. Raffaella Soave (raffaella.soave@scitec.cnr.it). My contributions dealt with theoretical and experimental studies of the crystallographic structure and chemical bonding of small/medium-size molecules of biological and pharmacological interest. I am also studying problems related to solid-state polymorphism of bioactive compounds, in the context of the wider crystal structure prediction (CSP) problem.

International Collaborations

From 2010 to 2019, I was a senior staff member of **the Center for Materials Crystallography** (CMC) led by Prof. Bo Brummerstedt Iversen at **Århus, Denmark**. I contributed to develop charge density-based methods for studying chemical bonding, non-covalent interactions, electronic structure and transmission of spin information in solids. I also applied statistical and computational tools to large crystallographic databases to disentangle which factors are primarily involved in the most crucial steps of the crystallization process, such as the choice between homomolecular and heteromolecular recognition, the relative importance of weak hydrogen bonds and the likelihood of spontaneous resolution. The final goal was to provide crystal chemists with a comprehensive view of the structural and energetic landscape of recurring motifs in crystal structures, out of which one might derive hints on the choice of promising compounds to guide the synthetic approach toward organic materials with the desired properties.

CMC has provided full funding for the following five PhD students which attended, or are now attending, the Doctorate School in Chemistry at the Università degli Studi di Milano. They all worked under my direct supervision as Tutor.

Giovanna Bruno (XXXIV cycle, 2018-2021)
Francesca Menescardi (XXXIII cycle, 2017-2020)
Giovanni Macetti (XXXI cycle, 2015–2018)
Ahmed M. Orlando (XVIII cycle, 2012–2015)
Gabriele Saleh (XXVI cycle, 2010–2013)

Scientific associations

From 2019 (until 12/31/2023) I am associated with the **National Institute of Nuclear Physics - Frascati National Laboratories** in the context of a research project for innovative perovskite-based sensors.

I have been associated with the **Center for Materials Crystallography (CMC) in Århus (DK)** led by prof. Bo Brummerstedt Iversen from 2010 to 2019. The CMC was an international research center funded by the Danish National Research Foundation, the Danish equivalent of the Italian CNR. Together with Drs. Carlo Gatti, Fausto Cargnoni and Davide Ceresoli of the CNR-ISTM, I participated in the Italian workgroup of the Centre. The CMC has fully funded 5 PhD scholarships under my responsibility at the PhD School of Chemistry of the University of Milan.

In 2011-2014 and 2017-2019 I was associated with the **Institute of Molecular Sciences and Technologies** (ISTM) of the National Research Council (CNR) in the framework of solid state research projects of the Department of Chemical Sciences and Materials Technologies.

Since 2007 I have been a member of the **Italian Crystallography Association**, a non-profit organization that aims to promote crystallography in Italy in all its educational and scientific aspects.

Editorial board membership

Since 2021, I have been a **member of the Editorial Board** of **Structural Chemistry** (Springer, Impact Factor = 1.795, https://www.springer.com/journal/11224/editors).

I was **Guest Editor** for 2 special issues of the open access journal **Crystals** (MDPI, Impact Factor = 2.589) dedicated to crystallization methods in gel or gel-like systems (https://www.mdpi.com/journal/crystals/special_issues/Crystal_Growth_Gels) and electron density (https://www.mdpi.com/journal/crystals/special_issues/charge_density).

Menagement activities

2018-2020: Member of the **Teaching Board** of the Teaching Coordination Council of the Chemistry Degrees at Università degli Studi di Milano.

2012-2017: Member of the **Instrumentation and Technical Gas Commission** of the Department of Chemistry.

2017-2023: Chair of the **Instrumentation and Technical Gas Commission** of the Department of Chemistry.

2019-2023: Member of the **steering board of the Analysis Laboratory** of the Department of Chemistry.

2023-present: Member of the **Scientific Committee** of the COSPECT Unitech technological platform at Università degli Studi di Milano.

Competitions and Evaluation Commissions

In 2024 I participated as designed member in an **internal evaluation procedure** for the career advancement to Associate Professor of a tenure track researcher (RTD-B) at the Chemistry Department at Università degli Studi di Milano.

In 2022 I participated as a designed member in a **comparative evaluation procedure** for the appointment of a type A fixed-term researcher (RTD-A) at the Chemistry Department at Università degli Studi di Milano.

In 2022 I participated in a **European tender commission** for the supply of a single crystal X-ray diffractometer framed in the Unitech COSPECT platform (Procedure SGa 22_446 – G00378; tender specification: 500 k€).

In 2021 I was a member of the **evaluation commission** for the awarding of the prize to the crystallographic thesis doctoral dissertation bestowed by the Italian crystallography association (AIC). I evaluated all the presented 7 PhD thesis works.

As a member of the teaching board of the PhD school in Chemistry, I participate to the evaluation procedure of the PhD students. I am also the referee of various PhD dissertations and I serve as a member in the Evaluation Committee of final PhD defenses.

Review and evaluation activities

I am reviewer of numerous international journals, including: CrystEngComm, Crystal Growth Des., Acta Crystallographica, Physical Chemistry Chemical Physics, Scientific Reports, Chemistry – A European Journal, Dalton Transaction, Solar Energy Materials and Solar Cells, Nanomaterials, RSC Advances, Advanced materials.

I evaluated 1 research project for the National Science Foundation (USA), 2 projects for the Austrian Science Fund (AT) ("stand alone" and "Lise Meitner" programs), 1 beamtime application for the Stanford synchrotron (SLAC, USA) and 1 project for the Italian Ministry of University and Research ("FISR" programme).

Appointment as an expert referee for the (VQR - valutazione della qualità della ricerca). I am currently serving as a referee on behalf of the Italian University Ministry to evaluate papers according to the research quality assessment procedure.

Congress Organization

- ICG2017 – Italian Crystal Growth Conference, Milano (Italy), 20-21/11/2017 (**Co-chair**) (http://sites.unimi.it/ICG2017/)
- SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities, S. Margherita di Pula (CA), Italy, 7-12/06/2015 (**Organizing Commettee**) (http://www.sagamorexviii.org/)
- ECDM-5 *European Charge Density Meeting*, Gravedona (CO), Italy, 6-11/06/2008 (**Organizing Committee**) (http://ecdm5.istm.cnr.it/)

Invited publications

- Invited contribution for a book Chapter in the Elsevier book series Reference Module in Chemistry, Molecular Science and Chemical Engineering, **2023** (DOI; 10.1016/B978-0-12-821978-2.00107-0)
- Invited contribution for **CrystEngComm**, **2022** (DOI: 10.1039/D2CE00957A)
- New Talent themed issue for **CrystEngComm**, **2018** (DOI: 10.1039/C8CE00674A)
- Margaret C. (Peggy) Etter Virtual Memorial Issue per **Crystal Growth & Design**, **2016** (DOI: 10.1021/acs.cgd.5b00442).
- Focus issue on Charge, Spin and Momentum Densities: SAGAMORE XVIII per **Physica Scripta**, **2016** (DOI: 10.1088/0031-8949/91/2/023001)

Teaching and Student Service

PhD-level Courses:

I have been a member of the Academic Board of the PhD School in Chemistry from 2008-2009 and from 2013-present.

Organization of PhD Courses:

- **2013** Taking a glance on ultrasmall and ultrafast worlds: time-resolved and free electron laser probes for chemical applications

- **2017** Discovering molecular recognition and self-assembling through the lenses of non-covalent interactions;

- **2019** Making experiment and theory talking together: A multidisciplinary approach for materials science

Master-Level degree Courses

2007-present: Responsible of the optional course on "**Crystal Chemistry**" (6 ECTS) for the Master's Degree in Chemical Sciences of the Università degli Studi di Milano.

2012-2023: Teacher of the optional course on **"Chemical Physical Methods for the study of the Structure of molecular and nanostructured systems"** (3 ECTS) for the Master's Degree in Chemical Sciences of the Università degli Studi di Milano.

2007-2020: Responsible for the fundamental course on **"Rational Design and structural characterization of bioactive molecules"** (note: over the years, this course has changed its name several times) for the Master's Degree in Molecular Biotechnologies and Bioinformatics dell'Università degli Studi di Milano (3 ECTS)

Bachelor-Level degree Courses:

2023-present: Responsible for the fundamental course on **"Physical Chemistry 1 / Laboratory of Physical Chemistry 1"** (12 ECTS) for the Bachelor's Degree in Chemical Sciences of the Università degli Studi di Milano. My commitment is related to the 6 credits of frontal lessons.

2023-present: Responsible of the optional course on **"Physical Chemistry of Materials"** (3 ECTS) for the Bachelor's Degree in Chemical Sciences of the Università degli Studi di Milano.

2021-2022, Responsible of the fundamental course on **"Physical Chemistry Laboratory**, Course A" (6 ECTS) for the Bachelor's Degree in Chemical Sciences of the Università degli Studi di Milano.

Since 2007, I have been carrying out student assistance activities (co-teaching) in practical laboratories of the Three-year Degree in Chemistry (Physical Chemistry Laboratory I and Physical Chemistry Laboratory II).

Evaluation Activities:

- 2015-2019: member of the Commission for Access to the Master's Degree in Chemical Sciences
- 2020-today: member of the Commission for Access to the Master's Degree in Industrial Chemistry

Third Mission and Orientation Activities

(1) 2011–2013. On behalf of the Orientation Commission, as part of the initiatives of the "Progetto Lauree Scientifiche", I organized and coordinated the "Energy Laboratory". This workshop, always held in the month of February (1 week), aims to illustrate different chemical and electrochemical strategies for energy conversion solar into electricity. More than 10 secondary schools were involved for a total of almost 400 students.

(2) 2011–2014. Also within the "Progetto Lauree Scientifiche", I contributed to coordinate the physical chemistry experiences of the interdisciplinary Summer School "Marinella Ferrari", held in the second week of June, for students of high school.

(3) 13-14 March 2012: Setting up of a stand with practical demonstrations on energy conversion at the Civic Aquarium of Milan, on the occasion of the initiative "interactive chemistry laboratories" organized as part of "L'Avventura della Scienza".

(4) February-May 2014: Coordination of the "Cristalli" activity in the field of the "Science Under 18" initiative aimed at high school students. About 60 students were involved, who attended introductory seminars at the Department of Chemistry, obtained crystals of ammonium phosphate through educational kits, and presented the results of their experiments in a stand in the honour courtyard at Università degli Studi di Milano.

(5) 2014. Preparation and curation of the exhibition “Cristalli! in Unimi”, organized as part of the initiatives of the Italian Crystallography Association in the context of celebrations for the International Year of Crystallography.

(6) November 28, 2014. Seminar "Signals from the invisible: a brief history of diffraction”, presented at the Civic Museum of Natural History in Milan col patronage of the Lombard Mineralogical Group - Italian Association of Mineralogy, as part of the initiatives for the International Year of Crystallography.

(7) February 27, 2015: Seminar "Brief introduction to crystallography" as part of “Progetto Lauree Scientifiche”

(8) May 19, 2017. Seminar "Signals from the invisible: a brief history of diffraction”, presented at the Levi Auditorium in Milan as part of the PLS event "Waves, Minerals and Crystals: History and Applications" during the award ceremony of the 2nd Crystal Growth National Competition organized by the Italian Crystallography Association.

(9) November 22, 2019. Seminar "Mendeleev: a map of everything", presented in Città Studi for the event 150 years of the Periodic Table of the Elements, organized under the patronage of the Department of Earth Sciences and Department of Chemistry (Università degli Studi di Milano), with the Department of Materials Sciences at the Università degli Studi di Milano-Bicocca.

Milano, 24/04/2024

Leonardo Lo Presti

Prof. Leonardo Lo Presti

Full Publication List ("*" marks the corresponding Author)

1. Giovanni Macetti, Luca Sironi, Costanza Rovida, Ilaria Geremia, Raffaella Soave*, **Leonardo Lo Presti***, On the solubility of azodicarbonamide in water/DMSO mixtures: an experimental and computational study. Royal Society Open Science 2024, *Accepted*.
2. Marta Papis, Sara Colombo, **Leonardo Lo Presti**, Giovanni Poli, Gianluigi Broggini, Julie Oble, Camilla Loro*, Palladium-Catalyzed/Mn(OAc)3-Mediated 1,2-Diazidation and 1,2-Acetoxy/Hydroxylation of N-Allyl Sulfonamides, Advanced Synthesis and Catalysis, 2024, *Accepted*.
3. Marta Papis, Raffaella Bucci, Alessandro Contini, Maria Luisa Gelmi, **Leonardo Lo Presti**, Giovanni Poli, Gianluigi Broggini, and Camilla Loro*. Phosphine-Catalyzed Domino Regio- and Stereo-Selective Hexamerization of 2-(Bromomethyl)acrylates to 1,2-Bis(cyclohexenyl)ethenyl Derivatives. Organic Letters 2023, 25, 7380–7384 DOI: 10.1021/acs.orglett.3c02836
4. Luca Sironi, Giovanni Macetti, **Leonardo Lo Presti***. Molecular Dynamics Investigation of Benzoic Acid in Confined Spaces. Physical Chemistry Chemical Physics 2023, 25, 28006-28019. DOI: 10.1039/D3CP02886K
5. Daniela Meroni, Carolina Cionti, Lucia Silvestrini, Noga Gal, Marco Cazzaniga, Michele Ceotto, Giacoo Buccella, **Leonardo Lo Presti***, Giuseppe Cappelletti. Oxygen vacancies in the Spotlight: On the engineering of intrinsic defects in highly defective TiO2 photocatalysts. Journal of Photochemistry & Photobiology, A: Chemistry 2023, 444, 114916. DOI: 10.1016/j.jphotochem.2023.114916
6. Ilenia Viola*, Fabio Matteocci, Luisa De Marco*, **Leonardo Lo Presti**, Silvia Rizzato, Simona Sennato, Alessandra Zizzari, Valentina Arima, Antonio De Santis, Chiara Rovelli, Silvio Morganti, Matthias Auf der Maur, Marianna Testa*. Microfluidic-Assisted Growth of Perovskite Single Crystals for Photodetectors. Advanced Materials Technologies, 2023, 2300023, DOI: 10.1002/admt.202300023
7. Luca Sironi, Silvia Rizzato, **Leonardo Lo Presti***. Why Is α-D-Glucose Monomorphic? Insights from Accurate Experimental Charge Density at 90 K. Cryst. Growth Des. 2022, 22, 11, 6627–6638, DOI: 10.1021/acs.cgd.2c00846
8. Marco Manenti, Simone Gusmini, **Leonardo Lo Presti**, Giorgio Molteni & Alessandra Silvani*. Enantiopure β-isocyano-boronic esters: synthesis and exploitation in isocyanide-based multicomponent reactions. Molecular Diversity 2022, DOI: 10.1007/s11030-022-10549-8.
9. Domenica Marabello*, Paola Antoniotti, Paola Benzi, Carlo Canepa, Elena Cariati, Alma Cioci, **Leonardo Lo Presti**. Second Harmonic Generation Behavior of Two New d-Ribose/d-Fructose and Metal Halogenide-Based Coordination Compounds and Comparison to d-Fructose and d-Galactose Analogues: An Experimental and Theoretical Approach. Cryst. Growth Des. 2022, 22, 10, 5923–5934. DOI: 10.1021/acs.cgd.2c00560
10. Riccardo Destro, Mario Barzaghi, Raffaella Soave, Pietro Roversi, **Leonardo Lo Presti***. Accurate experimental characterization of the labile N–Cl bond in N-chloro-N′-(p-fluorophenyl)-benzamidine crystal at 17.5 K. CrystEngComm 2022,24, 6215-6225. DOI: 10.1039/D2CE00957A
11. Raffaella Bucci, Francesco Vaghi, Davide Di Lorenzo, Francesco Anastasi, Gianluigi Broggini, **Leonardo Lo Presti**, Alessandro Contini, Maria Luisa Gelmi*. A Non-coded $\beta^{2,2}$-Amino Acid with Isoxazoline Core Able to Stabilize Peptides Folding through an

Unprecedented Hydrogen Bond. European Journal of Chemistry, 39, e202200601. DOI: 10.1002/ejoc.202200601

12. Marco Manenti, Simone Gusmini, **Leonardo Lo Presti**, Alessandra Silvani*. Exploiting Enantiopure β-Amino Boronic Acids in Isocyanide-Based Multicomponent Reactions. European Journal of Organic Chemistry, 2022, e202200435. DOI: 10.1002/ejoc.202200435
13. Paola Marzullo, Alice Maiocchi, Giuseppe Paladino, Umberto Ciriello, **Leonardo Lo Presti**, Daniele Passarella*, Total Synthesis of (−)-Cannabidiol-C_4, European Journal of Organic Chemistry, 2022, e202200392, DOI: 10.1002/ejoc.202200392
14. Camilla Loro, Letizia Molteni, Marta Papis, **Leonardo Lo Presti**, Francesca Foschi, Egle M. Beccalli,* Gianluigi Broggini*. Non-Decarboxylative Ruthenium-Catalyzed Rearrangement of 4-Alkylidene-isoxazol-5-ones to Pyrazole- and Isoxazole-4-carboxylic Acids. Org Lett. 2022, 24, 3092–3096. DOI: 10.1021/acs.orglett.2c01135
15. Marco Manenti, **Leonardo Lo Presti**, Giorgio Molteni, Alessandra Silvani*. Unexpected chiral vicinal tetrasubstituted diamines via borylcopper-mediated homocoupling of isatin imines. Beilstein J Org Chem. 2022, 18, 303-308. DOI: 10.3762/bjoc.18.34
16. **Leonardo Lo Presti***, Silvia Rizzato, Angelo Gavezzotti. Kinetic-Bias Model for the Dynamic Simulation of Molecular Aggregation. The Liquid, Solute, Solvated-Nanodrop, and Solvated-Nanocrystal States of Benzoic Acid. Cryst. Growth Des. 2022, 22, 3, 1857–1866. DOI: 10.1021/acs.cgd.1c01410
17. Camilla Loro, Letizia Molteni, Marta Papis, Egle M. Beccalli, Donatella Nava, **Leonardo Lo Presti**, Stefano Brenna, Gioele Colombo, Francesca Foschi, and Gianluigi Broggini*. Direct Synthesis of Fluorescent Oxazolo-phenoxazines by Copper-Catalyzed/Hypervalent Iodine(III)-Mediated Dimerization/Cyclization of 2-Benzylamino-phenols. J. Org. Chem. 2022, 87, 2, 1032–1042. DOI: 10.1021/acs.joc.1c02329
18. Angelo Gavezzotti*, **Leonardo Lo Presti**, Silvia Rizzato. Molecular Dynamics simulation of organic materials: Structure, potentials and the MiCMoS computer platform. CrystEngComm, 2022,24, 922-930. DOI: 10.1039/D1CE01360B
19. Sabrina Giofrè, Manfred Keller, **Leonardo Lo Presti**, Egle M. Beccalli*, Letizia Molteni. Switchable Oxidative Reactions of N -allyl-2-Aminophenols: Palladium-Catalyzed Alkoxyacyloxylation vs an Intramolecular Diels–Alder Reaction. Org. Lett. 2021, 23, 20, 7698–7702. DOI: 10.1021/acs.orglett.1c02539
20. Sabrina Giofrè, Letizia Molteni, Donatella Nava, **Leonardo Lo Presti**, Egle Maria Beccalli*. Enantio- and Regioselective Palladium(II)-Catalyzed Dioxygenation of (Aza)-Alkenols. Angewandte Chemie Int. Edition, 2021, 60, 21723-21727, DOI: 10.1002/anie.202109312
21. Marco Manenti, Stefano Gazzotti, **Leonardo Lo Presti**, Giorgio Molteni, Alessandra Silvani*. Highly diastereoselective entry to chiral oxindole-based β-amino boronic acids and spiro derivatives. Org. Biomol. Chem., 2021,19, 7211-7216, DOI: 10.1039/D1OB01303C
22. Domenica Marabello*, Paola Antoniotti, Paola Benzi, Fabio Beccari, Carlo Canepa, Elena Cariati, Alma Cioci, **Leonardo Lo Presti**. Crystal structure or chemical composition of salt–sugar-based metal–organic frameworks: what are the nonlinear optical properties due to? Acta Crystallogr. 2021, B77, 506–514. DOI: 10.1107/S2052520621004637
23. Riccardo Destro*, Pietro Roversi, Mario Barzaghi, **Leonardo Lo Presti**. Anharmonic Thermal Motion Modelling in the Experimental XRD Charge Density Determination of 1-Methyluracil at T = 23 K. Molecules (MDPI), 2021, 26(11), 3075. DOI: 10.3390/molecules26113075

24. **Leonardo Lo Presti**, Valentina Pifferi, Giovanni Di Liberto, Giuseppe Cappelletti, Luigi Falciola, Giuseppina Cerrato, Michele Ceotto*. Direct measurement and modeling of spontaneous charge migration across anatase–brookite nanoheterojunctions. J. Mater. Chem. A, 2021,9, 7782-7790. DOI: 10.1039/D1TA01040A

25. **Leonardo Lo Presti**, Jacopo Parravicini*, Raffaella Soave, Gianbattista Parravicini, Michele Mauri, Laura Loconte, Fabrizio Di Mei, Ludovica Falsi, Luca Tartara, Simona Binetti, Aharon J. Agranat, and Eugenio DelRe. Observation of an exotic lattice structure in the transparent $KTa_{1-x}Nb_xO_3$ perovskite supercrystal. Physical Review B 2020, 102, 214110. DOI: 10.1103/PhysRevB.102.214110

26. Silvia Rizzato, Angelo Gavezzotti, **Leonardo Lo Presti***. Molecular Dynamics Simulation of Molecular Crystals under Anisotropic Compression: Bulk and Directional Effects in Anthracene and Paracetamol. Cryst. Growth Des. 2020, 20, 11, 7421–7428. DOI: 10.1021/acs.cgd.0c01098

27. Riccardo Destro*, Pietro Roversi, Raffaella Soave, Arjan Hovestad, **Leonardo Lo Presti**. Experimental Charge Density Analysis and Electrostatic Properties of Crystalline 1,3-Bis(Dimethylamino)Squaraine and Its Dihydrate from Low Temperature (T = 18 and 20 K) XRD Data. Crystals (MDPI) 2020, 10(10), 894. DOI: 10.3390/cryst10100894

28. Giovanna Bruno, Giovanni Macetti, **Leonardo Lo Presti**, Carlo Gatti*. Spin Density Topology. Molecules (MDPI) 2020, 25(15), 3537. DOI: 10.3390/molecules25153537

29. Giada Finocchio, Silvia Rizzato, Giovanni Macetti, Gers Tusha, **Leonardo Lo Presti***: Unravelling the Chemistry of the [Cu(4,7-Dichloroquinoline)2Br2]2 Dimeric Complex through Structural Analysis: A Borderline Ligand Field Case. Crystals (MDPI), 2020,10,477, DOI: 10.3390/cryst10060477

30. Angelo Gavezzotti*, Silvia Rizzato, **Leonardo Lo Presti**. Mining the Cambridge Database for theoretical chemistry. Mi-LJC: a new set of Lennard-Jones‑Coulomb atom‑atom potentials for the computer simulation of organic condensed matter. CrystEngComm 2020, DOI: 10.1039/D0CE00334D

31. Emanuele Bassini, Stefano Gazzotti, Filomena Sannio, **Leonardo Lo Presti**, Jacopo Sgrignani, Jean-Denis Docquier, Giovanni Grazioso, Alessandra Silvani*. Isonitrile-Based Multicomponent Synthesis of β-Amino Boronic Acids as β-Lactamase Inhibitors. Antibiotics (Basel) 2020 May 12;9(5):249. DOI: 10.3390/antibiotics9050249

32. Angelo Gavezzotti, **Leonardo Lo Presti***, Molecular dynamics simulation of organic crystals: introducing the CLP-dyncry environment. J. Appl. Cryst. 2019, 52, 1253-1263. DOI: 10.1107/S1600576719012238

33. **Leonardo Lo Presti**, Massimo Moret, Silvia Rizzato*, Phase Stability and Morphology of Gel Grown Crystals: The Case of CdCl 2 -bpp Polymeric System. Crystals 2019, 9: 363, DOI: 10.3390/cryst9070363

34. Francesca Foschi, Camilla Loro, Roberto Sala, Oble Julie, **Leonardo Lo Presti**, Egle M. Beccalli, Giovanni Poli, Gianluigi Broggini*, Intramolecular Aminoazidation of Unactivated Terminal Alkenes by Palladium-Catalyzed Reactions with Hydrogen Peroxideas the Oxidant. Organic Letters 2020, 22, 4, 1402-1406, DOI:10.1021/acs.orglett.0c00010

35. Stefano Gazzotti, Marco Manenti, **Leonardo Lo Presti** and Alessandra Silvani*: Allylation of isatin-derived N-Boc-hydrazones followed by Pd-catalyzed carboamination reaction: an entry to 3-spiro-pyrazolidyl-oxindoles. RSC Advances, 9 2019, 37788‑3788, DOI: 10.1039/c9ra07712jù

36. Elisa Bonandi, Paola Marzullo, Francesca Foschi, Dario Perdicchia, **Leonardo Lo Presti**, Maurizio Sironi, Stefano Pieraccini, Guido Gambacorta, Joern Saupe, Lisa Dalla Via, Daniele Passarella*, Stereodivergent Diversity-Oriented Synthesis: Exploiting the Versatility of 2-Piperidine Ethanol. European Journal of Organic Chemistry, 25, 2019, 4013‑4019, DOI: 10.1002/ejoc.201900461

37. Sabrina Giofre, Roberto Sala, Egle Maria Beccalli, **Leonardo Lo Presti**, Gianluigi Broggini*. Iodoamination of Alkenyl Sulfonamides by Potassium Iodide and Hydrogen Peroxide in Aqueous Medium. Helvetica Chimica Acta, 102, 2019, e190088, DOI: 10.1002/hlca.201900088

38. Sabrina Giofre, Egle M. Beccalli *, Francesca Foschi, Concetta La Rosa, **Leonardo Lo Presti**, Michael S. Christodoulou. Chemo- and Regioselective Palladium(II)-Catalyzed Aminoarylation of N-Allylureas Providing 4-Arylmethyl Imidazolidinones. Synthesis 51, 2019, 3462-3470. DOI: 10.1055/s-0037-1611539

39. Domenica Marabello*, Paola Antoniotti, Paola Benzi, Elena Cariati, **Leonardo Lo Presti**, Carlo Canepa: Developing new SrI2 and β-D-fructopyranose-based metal–organic frameworks with nonlinear optical properties. Acta Crystallographica Section B 75:210-218. DOI: 10.1107/S2052520619001951

40. 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 Piperaquine. Cryst. Growth Des. 2019, 19, 1399-1410, DOI: 10.1021/acs.cgd.8b01794

41. 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

42. 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

43. 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 Broggini, 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

44. 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

45. Giulia Rainoldi, Giordano Lesma, Claudia Picozzi, **Leonardo Lo Presti**, Alessandra Silvani*: One step access to oxindole-based β-lactams through Ugi four-center threecomponent reaction. RSC Advances 2018, 8, 34903-34910, DOI: 10.1039/C8RA08165D

46. **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)

47. 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 – M2+ triflate system. CrystEngComm, 2018,20, 3784-3795. DOI: 10.1039/C8CE00653

48. Cinzia Colombo*, Črtomir 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

49. 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 Comb. Sci., 2018, 20 (2), 98‑105, DOI: 10.1021/acscombsci.7b00179

50. 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

51. 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 10/2017, 2(31):10295-10299, DOI: 10.1002/slct.201702154

52. Giovanni Di Liberto, Valentina Pifferi, **Leonardo Lo Presti***, Michele Ceotto*, Luigi Falciola*: An Atomistic Explanation for Interlayer Charge Transfer in Metal-Semiconductor Nanocomposites: The Case of Silver and Anatase. J. Phys. Chem. Lett. 10/2017, 8, 5372-5377, DOI; 10.1021/acs.jpclett.7b02555

53. 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 ($Mg_3Al_2Si_3O_{12}$) 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

54. 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

55. 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

56. 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 TiO_2-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

57. Michael S Christodoulou, Fabiana Caporuscio, Valentina Restelli, Luca Carlino, Giuseppe Cannazza, Elisa Costanzi, Cinzia Citti, **Leonardo Lo Presti**, Pasquale Pisani, Roberto Battistutta, Massimo Broggini, Daniele Passarella, Giulio Rastelli*: Probing an Allosteric Pocket of CDK2 with Small Molecules. ChemMedChem 01/2017; 12:33-41., DOI:10.1002/cmdc.201600474

58. 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

59. 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

60. 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

61. 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

62. Michael S. Christodoulou*, Mikel Zarate, Francesca Ricci, Giovanna Damia, Stefano Pieraccini, Federico Dapiaggi, Maurizio Sironi, **Leonardo Lo Presti**, Aida Nelly Garcia-Argaez, 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

63. 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

64. 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

65. 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

66. 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

67. 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)., DOI:10.1021/acs.cgd.5b00442

68. 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. Medicinal Chemistry Communication 05/2015; 6(7):1260-1266., DOI:10.1039/C5MD00159E

69. 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

70. 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

71. 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
72. **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
73. 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
74. 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
75. **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
76. 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
77. **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
78. 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
79. 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
80. Gabriele Saleh*, **Leonardo Lo Presti**, Carlo Gatti, Davide Ceresoli: NCImilano: An electrondensity-based code for the study of noncovalent interactions. Journal of Applied Crystallography 10/2013; 46(5):1513-1517., DOI:10.1107/S0021889813020098
81. 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 Tc = 122.6 K. Crystal Growth & Design 08/2013; 13(10-10):4571-4582., DOI:10.1021/cg401123s

82. 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
83. 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
84. 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
85. Gabriele Saleh, Carlo Gatti*, **Leonardo Lo Presti***, Julia Contreras-Garcia: 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
86. 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
87. 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
88. 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 TiO 2: Combined DFT and EXAFS approach. The Journal of Physical Chemistry C 01/2012; 116(2):1764-1771., DOI:10.1021/jp2097636
89. **Leonardo Lo Presti***, Mattia Allieta, Marco Scavini, Paolo Ghigna, Laura Loconte, Valerio Scagnoli, Michela Brunelli: Crystal structure and structural phase transitions in the $GdBaCo_2O_{5.0}$ cobaltite. Physical review. B, Condensed matter 09/2011; 84(10)., DOI:10.1103/PhysRevB.84.104107
90. **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
91. 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
92. 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

93. 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

94. .**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

95. 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 Δ2-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

96. Ahmed M Orlando, **Leonardo Lo Presti***, Raffaella Soave: A new monoclinic polymorph of 3-diethyl-amino-4-(4-meth-oxy-phen-yl)-1,1-dioxo-4H-1λ,2-thia-zete-4-carbonitrile. Acta Crystallographica Section E Structure Reports Online 08/2010; 66(Pt 8):o2032-3., DOI:10.1107/S1600536810027558

97. 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 thiiranium ion into thietanium ion. Physical Chemistry Chemical Physics 10/2009; 11(33):7181-8., DOI:10.1039/b901928f

98. **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

99. **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

100. **Leonardo Lo Presti***, Riccardo Destro: Experimental and theoretical charge density distribution of the colossal magnetoresistive transition metal sulfide $FeCr_2S_4$. The Journal of Chemical Physics 02/2008; 128(4):044710., DOI:10.1063/1.2822160

101. **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 (C 12 H 12 O 5). The Journal of Physical Chemistry B 04/2006; 110(12):6405-14.,DOI:10.1021/jp056823y

102. **Leonardo Lo Presti**, Donatella Invernizzi, Raffaella Soave, Riccardo Destro*: Looking for structural phase transitions in the colossal magnetoresistive thiospinel $FeCr_2S_4$ by a multitemperature single-crystal X-ray diffraction study. Chemical Physics Letters 11/2005; 416(1- 3):28-32., DOI:10.1016/j.cplett.2005.09.037

103. 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 ($C_{30}H_{30}N_6O_3S$) atT=17 K. Chemistry: A European Journal 2005; 11(16):4621-34., DOI:10.1002/chem.200400964

104. 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

105. **Leonardo Lo Presti**, Raffaella Soave*, Riccardo Destro: The Fungal Metabolite Austdiol. Acta Crystallographica Section C Crystal Structure Communications 08/2003; 59:O199-201., DOI:10.1002/chin.200334211

106. 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 2002; 58(25):5173-5178., DOI:10.1016/S0040-4020(02)00445-3

Book Chapters:

1. Giovanni Macetti, Luca Sironi, Leonardo Lo Presti. Classical Molecular Dynamics Simulation of Molecular Crystals and Materials: Old Lessons and New Perspectives. Elsevier Reference Collection in Chemistry, Molecular Sciences and Chemical Engineering (2023). DOI: 10.1016/B978-0-12-821978-2.00107-0
2. 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)
3. 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).

Milano, 07/07/2023

Leonardo Lo Presti