Leonardo Lo Presti

List of Publications by Year
in descending order

102	2,139	257450	276875
papers	citations	24 h-index	41 g-index

106	106	106	2593
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Direct Synthesis of Fluorescent Oxazolo-phenoxazines by Copper-Catalyzed/Hypervalent Iodine(III)-Mediated Dimerization/Cyclization of 2-Benzylamino-phenols. Journal of Organic Chemistry, 2022, 87, 1032-1042.	3.2	10
2	Molecular dynamics simulation of organic materials: structure, potentials and the MiCMoS computer platform. CrystEngComm, 2022, 24, 922-930.	2.6	8
3	Kinetic-Bias Model for the Dynamic Simulation of Molecular Aggregation. The Liquid, Solute, Solvated-Nanodrop, and Solvated-Nanocrystal States of Benzoic Acid. Crystal Growth and Design, 2022, 22, 1857-1866.	3.0	5
4	Unexpected chiral vicinal tetrasubstituted diamines via borylcopper-mediated homocoupling of isatin imines. Beilstein Journal of Organic Chemistry, 2022, 18, 303-308.	2.2	3
5	Non-Decarboxylative Ruthenium-Catalyzed Rearrangement of 4-Alkylidene-isoxazol-5-ones to Pyrazole- and Isoxazole-4-carboxylic Acids. Organic Letters, 2022, , .	4.6	8
6	Total Synthesis of (â^')â€Cannabidiolâ€C₄. European Journal of Organic Chemistry, 2022, 2022, .	2.4	6
7	Highly diastereoselective entry to chiral oxindole-based Î²-amino boronic acids and spiro derivatives. Organic and Biomolecular Chemistry, 2021, 19, 7211-7216.	2.8	4
8	Direct measurement and modeling of spontaneous charge migration across anataseâ€“brookite nanoheterojunctions. Journal of Materials Chemistry A, 2021, 9, 7782-7790.	10.3	14
9	Anharmonic Thermal Motion Modelling in the Experimental XRD Charge Density Determination of 1-Methyluracil at T = 23 K. Molecules, 2021, 26, 3075.	3.8	5
10	Crystal structure or chemical composition of saltâ€“sugar-based metalâ€“organic frameworks: what are the nonlinear optical properties due to?. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 506-514.	1.1	2
11	Switchable Oxidative Reactions of N-allyl-2-Aminophenols: Palladium-Catalyzed Alkoxyacyloxylation vs an Intramolecular Dielsâ€“Alder Reaction. Organic Letters, 2021, 23, 7698-7702.	4.6	10
12	Enantioâ€•and Regioselective Palladium(II)â€Catalyzed Dioxygenation of (Azaâ€)Alkenols. Angewandte Chemie, 2021, 133, 21891-21895.	2.0	2
13	Enantioâ€•and Regioselective Palladium(II)â€Catalyzed Dioxygenation of (Azaâ€)Alkenols. Angewandte Chemie - International Edition, 2021, 60, 21723-21727.	13.8	11
14	Molecular Dynamics Simulation of Molecular Crystals under Anisotropic Compression: Bulk and Directional Effects in Anthracene and Paracetamol. Crystal Growth and Design, 2020, 20, 7421-7428.	3.0	6
15	Spin Density Topology. Molecules, 2020, 25, 3537.	3.8	20
16	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, 2020, 10, 894.	2.2	1
17	Isonitrile-Based Multicomponent Synthesis of Î²-Amino Boronic Acids as Î²-Lactamase Inhibitors. Antibiotics, 2020, 9, 249.	3.7	12
18	Unravelling the Chemistry of the [Cu(4,7-Dichloroquinoline)2Br2]2 Dimeric Complex through Structural Analysis: A Borderline Ligand Field Case. Crystals, 2020, 10, 477.	2.2	3

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19	Intramolecular Aminoazidation of Unactivated Terminal Alkenes by Palladium-Catalyzed Reactions with Hydrogen Peroxide as the Oxidant. Organic Letters, 2020, 22, 1402-1406.	4.6	31
20	Mining the Cambridge Database for theoretical chemistry. Mi-LJC: a new set of Lennard-Jonesâ€“Coulomb atomâ€“atom potentials for the computer simulation of organic condensed matter. CrystEngComm, 2020, 22, 7350-7360.	2.6	17
21	Observation of an exotic lattice structure in the transparent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">K</mml:mi><mml:mi>Ta</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math> perovskite supercrystal. Physical Review B, 2020, 102, .	3.2	8
22	Developing new SrI₂ and Î²-<scp>D</scp>-fructopyranose-based metalâ€“organic frameworks with nonlinear optical properties. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 210-218.	1.1	4
23	Phase Stability and Morphology of Gel Grown Crystals: The Case of CdCl2-bpp Polymeric System. Crystals, 2019, 9, 363.	2.2	0
24	Dynamic simulation of liquid molecular nanoclusters: structure, stability and quantification of internal (pseudo)symmetries. New Journal of Chemistry, 2019, 43, 2077-2084.	2.8	11
25	Chemo- and Regioselective Palladium(II)-Catalyzed AminoarylÂation of N-Allylureas Providing 4-Arylmethyl Imidazolidinones. Synthesis, 2019, 51, 3462-3470.	2.3	10
26	Iodoamination of Alkenyl Sulfonamides by Potassium Iodide and Hydrogen Peroxide in Aqueous Medium. Helvetica Chimica Acta, 2019, 102, e1900088.	1.6	9
27	Stereodivergent Diversityâ€Oriented Synthesis: Exploiting the Versatility of 2â€Piperidine Ethanol. European Journal of Organic Chemistry, 2019, 2019, 4013-4019.	2.4	5
28	Molecular dynamics simulation of organic crystals: introducing the CLP-dyncry environment. Journal of Applied Crystallography, 2019, 52, 1253-1263.	4.5	17
29	Allylation of isatin-derived N-Boc-hydrazones followed by Pd-catalyzed carboamination reaction: an entry to 3-spiro-pyrazolidyl-oxindoles. RSC Advances, 2019, 9, 37788-37800.	3.6	3
30	Correlations of Crystal Structure and Solubility in Organic Salts: The Case of the Antiplasmodial Drug Piperaquine. Crystal Growth and Design, 2019, 19, 1399-1410.	3.0	13
31	CLPdyn: a cheap and reliable tool for molecular dynamics studies of organic molecules in the condensed phase. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e540-e540.	0.1	0
32	Sequential Multicomponent Strategy for the Diastereoselective Synthesis of Densely Functionalized Spirooxindole-Fused Thiazolidines. ACS Combinatorial Science, 2018, 20, 98-105.	3.8	22
33	Spin density accuracy and distribution in azido Cu(II) complexes: A source function analysis. Journal of Computational Chemistry, 2018, 39, 587-603.	3.3	9
34	A variable-temperature X-ray diffraction and theoretical study of conformational polymorphism in a complex organic molecule (DTC). RSC Advances, 2018, 8, 38445-38454.	3.6	8
35	One step access to oxindole-based Î²-lactams through Ugi four-center three-component reaction. RSC Advances, 2018, 8, 34903-34910.	3.6	20
36	Structureâ€“Activity Relationships of Hexahydrocyclopenta[c]quinoline Derivatives as Allosteric Inhibitors of CDK2 and EGFR. ChemMedChem, 2018, 13, 2627-2634.	3.2	23

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37	The TACO Puzzle: A Phase-Transition Mystery Revisited. Crystal Growth and Design, 2018, 18, 7219-7227.	3.0	5
38	Crystallization and structural properties of a family of isotopological 3D-networks: the case of a 4,4â€²-bipy ligandâ€“M2+ triflate system. CrystEngComm, 2018, 20, 3784-3795.	2.6	3
39	On the significance of weak hydrogen bonds in crystal packing: a large databank comparison of polymorphic structures. CrystEngComm, 2018, 20, 5976-5989.	2.6	29
40	Design and synthesis of constrained bicyclic molecules as candidate inhibitors of influenza A neuraminidase. PLoS ONE, 2018, 13, e0193623.	2.5	6
41	Two-component organic crystals without hydrogen bonding: structure and intermolecular interactions in bimolecular stacking. CrystEngComm, 2017, 19, 2413-2423.	2.6	30
42	A Close Look at the Structure of the TiO₂-APTES Interface in Hybrid Nanomaterials and Its Degradation Pathway: An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2017, 121, 430-440.	3.1	123
43	Atomistic Explanation for Interlayer Charge Transfer in Metalâ€“Semiconductor Nanocomposites: The Case of Silver and Anatase. Journal of Physical Chemistry Letters, 2017, 8, 5372-5377.	4.6	25
44	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, Crystal Engineering and Materials, 2017, 73, 565-583.	1.1	14
45	Synthesis of<scp>l</scp>-Tricholomic Acid Analogues and Pharmacological Characterization at Ionotropic Glutamate Receptors. ChemistrySelect, 2017, 2, 10295-10299.	1.5	3
46	Probing an Allosteric Pocket of CDK2 with Small Molecules. ChemMedChem, 2017, 12, 33-41.	3.2	21
47	Insights on spin-density delocalization/polarization mechanisms through the source function. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1434-C1434.	0.1	0
48	Anharmonic motionsversusdynamic disorder at the Mg ion from the charge densities in pyrope (Mg₃Al₂Si₃O₁₂) crystals at 30â€…K: six of one, half a dozen of the other. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 722-736.	1.1	12
49	4-(1,2-diarylbut-1-en-1-yl)isobutyranilide derivatives as inhibitors of topoisomerase II. European Journal of Medicinal Chemistry, 2016, 118, 79-89.	5.5	24
50	Building Blocks of Crystal Engineering: A Large-Database Study of the Intermolecular Approach between Câ€“H Donor Groups and O, N, Cl, or F Acceptors in Organic Crystals. Crystal Growth and Design, 2016, 16, 2952-2962.	3.0	57
51	Exploring Chemistry Through the Source Function for the Electron and the Electron Spin Densities. Challenges and Advances in Computational Chemistry and Physics, 2016, , 101-129.	0.6	3
52	Intermolecular Recognition of the Antimalarial Drug Chloroquine: A Quantum Theory of Atoms in Moleculesâ€“Density Functional Theory Investigation of the Hydrated Dihydrogen Phosphate Salt from the 103 K X-ray Structure. Crystal Growth and Design, 2016, 16, 6043-6054.	3.0	17
53	Highly diastereoselective entry into chiral spirooxindole-based 4-methyleneazetidines via formal [2+2] annulation reaction. Chemical Communications, 2016, 52, 11575-11578.	4.1	31
54	Facts and Factors in the Formation and Stability of Binary Crystals. Crystal Growth and Design, 2016, 16, 6095-6104.	3.0	43

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55	Source Function applied to experimental densities reveals subtle electron-delocalization effects and appraises their transferability properties in crystals. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 180-193.	1.1	24
56	On the molecular basis of the activity of the antimalarial drug chloroquine: EXAFS-assisted DFT evidence of a direct Feâ€“N bond with free heme in solution. Physica Scripta, 2016, 91, 023001.	2.5	7
57	Model peptides containing the 3-sulfanyl-norbornene amino acid, a conformationally constrained cysteine analogue effective inducer of 3₁₀-helix secondary structures. RSC Advances, 2015, 5, 32643-32656.	3.6	20
58	Synthesis of unusual isoxazoline containing Î² and Î³-dipeptides as potential glutamate receptor ligands. MedChemComm, 2015, 6, 1260-1266.	3.4	7
59	Theoretical Study of Chiral Carboxylic Acids. Structural and Energetic Aspects of Crystalline and Liquid States. Crystal Growth and Design, 2015, 15, 3792-3803.	3.0	64
60	Insights on spin polarization through the spin density source function. Chemical Science, 2015, 6, 3845-3852.	7.4	20
61	Impregnation versus Bulk Synthesis: How the Synthetic Route Affects the Photocatalytic Efficiency of Nb/Ta:N Codoped TiO₂ Nanomaterials. Journal of Physical Chemistry C, 2015, 119, 24104-24115.	3.1	36
62	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, 2015, 58, 7938-7948.	6.4	12
63	Energetics of non-covalent interactions from electron and energy density distributions. Computational and Theoretical Chemistry, 2015, 1053, 53-59.	2.5	64
64	Second Generation Nitrogen Doped Titania Nanoparticles: A Comprehensive Electronic and Microstructural Picture. Chinese Journal of Chemistry, 2014, 32, 1195-1213.	4.9	20
65	Rationalizing the Lacking of Inversion Symmetry in a Noncentrosymmetric Polar Racemate: An Experimental and Theoretical Study. Crystal Growth and Design, 2014, 14, 5822-5833.	3.0	17
66	Role of the Nitrogen Source in Determining Structure and Morphology of N-Doped Nanocrystalline TiO2. Journal of Physical Chemistry C, 2014, 118, 4797-4807.	3.1	33
67	Unraveling the Cooperative Mechanism of Visible-Light Absorption in Bulk N,Nb Codoped TiO₂ Powders of Nanomaterials. Journal of Physical Chemistry C, 2014, 118, 24152-24164.	3.1	47
68	Single Nâ€“C Bond Becomes Shorter than a Formally Double Nâ•C Bond in a Thiazete-1,1-dioxide Crystal: An Experimental and Theoretical Study of Strong Crystal Field Effects. Crystal Growth and Design, 2014, 14, 4418-4429.	3.0	11
69	Asymmetric Modular Synthesis of a Semirigid Dipeptide Mimetic by Cascade Cycloaddition/Ring Rearrangement and Borohydride Reduction. Journal of Organic Chemistry, 2014, 79, 3094-3102.	3.2	26
70	Insights on spin-polarization via the spin density Source Function. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C281-C281.	0.1	1
71	Decoding conformational polymorphism in organic substances. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C557-C557.	0.1	0
72	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, 2013, 19, 3490-3503.	3.3	18

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73	Competing Câ•OÂ·Â·Â·Câ•O, Câ€“HÂ·Â·Â·O, ClÂ·Â·Â·O, and ClÂ·Â·Â·Cl Interactions Governing the Structural Phase Transition of 2,6-Dichloro-p-benzoquinone atTc= 122.6 K. Crystal Growth and Design, 2013, 13, 4571-4582.	3.6	22
74	NCImilano: an electron-density-based code for the study of noncovalent interactions. Journal of Applied Crystallography, 2013, 46, 1513-1517.	4.5	50
75	Development of Rhodesain Inhibitors with a 3â€Bromoisoxazoline Warhead. ChemMedChem, 2013, 8, 2070-2076.	3.2	37
76	Charge ordering transition in GdBaCo2O5: Evidence of reentrant behavior. Physical Review B, 2013, 88, .	3.2	16
77	Evading Pgp Activity in Drug-Resistant Cancer Cells: A Structural and Functional Study of Antitubulin Furan Metotica Compounds. Molecular Cancer Therapeutics, 2012, 11, 1103-1111.	4.1	12
78	Non-covalent interaction via the reduced density gradient: Independent atom model vs experimental multipolar electron densities. Computational and Theoretical Chemistry, 2012, 998, 148-163.	2.5	164
79	Revealing Nonâ€covalent Interactions in Molecular Crystals through Their Experimental Electron Densities. Chemistry - A European Journal, 2012, 18, 15523-15536.	3.3	173
80	Role of Pr on the Semiconductor Properties of Nanotitania. An Experimental and First-Principles Investigation. Journal of Physical Chemistry C, 2012, 116, 23083-23093.	3.1	19
81	Synthesis and Biological Evaluation of CTP Synthetase Inhibitors as Potential Agents for the Treatment of African Trypanosomiasis. ChemMedChem, 2012, 7, 1623-1634.	3.2	29
82	About the Nitrogen Location in Nanocrystalline N-Doped TiO₂: Combined DFT and EXAFS Approach. Journal of Physical Chemistry C, 2012, 116, 1764-1771.	3.1	74
83	Rationalizing the Effect of Halogenation on the Molecular Structure of Simple Cyclobutene Derivatives by Topological Real-Space Analysis of Their Electron Density. Journal of Physical Chemistry A, 2011, 115, 12695-12707.	2.5	15
84	Revealing Electron Delocalization through the Source Function. Journal of Physical Chemistry A, 2011, 115, 12864-12878.	2.5	51
85	Multi-temperature Electron Density Studies. , 2011, , 659-696.		3
86	UV absorbing zwitterionic pyridinium-tetrazolate: exceptional transparency/optical nonlinearity trade-off. Chemical Communications, 2011, 47, 292-294.	4.1	20
87	Regioselective Preparation of Functionalized Isoxazoline Derivatives as Key Intermediates for the Synthesis of Selective N-Methyl-d-aspartate Receptor Antagonists. Synthesis, 2011, 2011, 1255-1260.	2.3	3
88	Crystal structure and structural phase transitions in the GdBaCo<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>5.0</mml:mn></mml:mrow></mml:msub></mml:math>cobaltite. Physical Review B, 2011, 84, .	3.2	17
89	Conformational polymorphism in a Schiff-base macrocyclic organic ligand: an experimental and theoretical study. Acta Crystallographica Section B: Structural Science, 2010, 66, 527-543.	1.8	13
90	A new monoclinic polymorph of 3-diethylamino-4-(4-methoxyphenyl)-1,1-dioxo-4H-1Î»6,2-thiazete-4-carbonitrile. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o2032-o2033.	0.2	2

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91	Synthesis of novel chiral Î”2-isoxazoline derivatives related to ABT-418 and estimation of their affinity at neuronal nicotinic acetylcholine receptor subtypes. European Journal of Medicinal Chemistry, 2010, 45, 5594-5601.	5.5	13
92	Using the Source Function descriptor to dampen the multipole model bias in charge density studies from X-ray structure factors refinements. Chemical Physics Letters, 2009, 476, 308-316.	2.6	25
93	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. Journal of Physical Chemistry A, 2009, 113, 3186-3196.	2.5	13
94	Detection and kinetics of the single-crystal to single-crystal complete transformation of a thiiranium ion into thietanium ion. Physical Chemistry Chemical Physics, 2009, 11, 7181.	2.8	7
95	Experimental and theoretical charge density distribution of the colossal magnetoresistive transition metal sulfide FeCr2S4. Journal of Chemical Physics, 2008, 128, 044710.	3.0	13
96	On the Interplay between CHÂ·Â·Â·O and OHÂ·Â·Â·O Interactions in Determining Crystal Packing and Molecular Conformation:Â An Experimental and Theoretical Charge Density Study of the Fungal Secondary Metabolite Austdiol (C12H12O5). Journal of Physical Chemistry B, 2006, 110, 6405-6414.	2.6	44
97	Looking for structural phase transitions in the colossal magnetoresistive thiospinel FeCr2S4 by a multi-temperature single-crystal X-ray diffraction study. Chemical Physics Letters, 2005, 416, 28-32.	2.6	11
98	Progress in the Understanding of Drug-Receptor Interactions, Part 1: Experimental Charge-Density Study of an Angiotensin II Receptor Antagonist (C30H30N6O3S) atT=17 K. Chemistry - A European Journal, 2005, 11, 4621-4634.	3.3	36
99	On the role of data quality in experimental charge-density studies. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 365-370.	0.3	18
100	The fungal metabolite austdiol. Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, o199-o201.	0.4	8
101	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, 5173-5178.	1.9	18
102	Isothiazoles. Part 13. Synthesis of Sulfamic Esters, [1,2]Thiazete S,Sâ€Dioxides, Benzo[e][1,2]thiazine S,Sâ€Dioxides or Triazoles by Reaction of Isothiazole Dioxides with Sodium Azide.. ChemInform, 2002, 33, 50-50.	0.0	0