

Leonardo Lo Presti

List of Publications by Year in descending order

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102
papers

2,139
citations

257450

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106
docs citations

106
times ranked

2593
citing authors

#	ARTICLE	IF	CITATIONS
1	Revealing Non-covalent Interactions in Molecular Crystals through Their Experimental Electron Densities. <i>Chemistry - A European Journal</i> , 2012, 18, 15523-15536.	3.3	173
2	Non-covalent interaction via the reduced density gradient: Independent atom model vs experimental multipolar electron densities. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 148-163.	2.5	164
3	A Close Look at the Structure of the TiO ₂ -APTES Interface in Hybrid Nanomaterials and Its Degradation Pathway: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 430-440.	3.1	123
4	About the Nitrogen Location in Nanocrystalline N-Doped TiO ₂ : Combined DFT and EXAFS Approach. <i>Journal of Physical Chemistry C</i> , 2012, 116, 1764-1771.	3.1	74
5	Theoretical Study of Chiral Carboxylic Acids. Structural and Energetic Aspects of Crystalline and Liquid States. <i>Crystal Growth and Design</i> , 2015, 15, 3792-3803.	3.0	64
6	Energetics of non-covalent interactions from electron and energy density distributions. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 53-59.	2.5	64
7	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. <i>Crystal Growth and Design</i> , 2016, 16, 2952-2962.	3.0	57
8	Revealing Electron Delocalization through the Source Function. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12864-12878.	2.5	51
9	<i>ncimilano</i> : an electron-density-based code for the study of noncovalent interactions. <i>Journal of Applied Crystallography</i> , 2013, 46, 1513-1517.	4.5	50
10	Unraveling the Cooperative Mechanism of Visible-Light Absorption in Bulk N,Nb Codoped TiO ₂ Powders of Nanomaterials. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24152-24164.	3.1	47
11	On the Interplay between CH \cdots O and OH \cdots 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). <i>Journal of Physical Chemistry B</i> , 2006, 110, 6405-6414.	2.6	44
12	Facts and Factors in the Formation and Stability of Binary Crystals. <i>Crystal Growth and Design</i> , 2016, 16, 6095-6104.	3.0	43
13	Development of Rhodesain Inhibitors with a Bromoisoxazoline Warhead. <i>ChemMedChem</i> , 2013, 8, 2070-2076.	3.2	37
14	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 ₆ O ₃ S) at T=17 K. <i>Chemistry - A European Journal</i> , 2005, 11, 4621-4634.	3.3	36
15	Impregnation versus Bulk Synthesis: How the Synthetic Route Affects the Photocatalytic Efficiency of Nb/Ta:N Codoped TiO ₂ Nanomaterials. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24104-24115.	3.1	36
16	Role of the Nitrogen Source in Determining Structure and Morphology of N-Doped Nanocrystalline TiO ₂ . <i>Journal of Physical Chemistry C</i> , 2014, 118, 4797-4807.	3.1	33
17	Highly diastereoselective entry into chiral spirooxindole-based 4-methyleneazetidines via formal [2+2] annulation reaction. <i>Chemical Communications</i> , 2016, 52, 11575-11578.	4.1	31
18	Intramolecular Aminoazidation of Unactivated Terminal Alkenes by Palladium-Catalyzed Reactions with Hydrogen Peroxide as the Oxidant. <i>Organic Letters</i> , 2020, 22, 1402-1406.	4.6	31

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19	Two-component organic crystals without hydrogen bonding: structure and intermolecular interactions in bimolecular stacking. <i>CrystEngComm</i> , 2017, 19, 2413-2423.	2.6	30
20	Synthesis and Biological Evaluation of CTP Synthetase Inhibitors as Potential Agents for the Treatment of African Trypanosomiasis. <i>ChemMedChem</i> , 2012, 7, 1623-1634.	3.2	29
21	On the significance of weak hydrogen bonds in crystal packing: a large databank comparison of polymorphic structures. <i>CrystEngComm</i> , 2018, 20, 5976-5989.	2.6	29
22	Asymmetric Modular Synthesis of a Semirigid Dipeptide Mimetic by Cascade Cycloaddition/Ring Rearrangement and Borohydride Reduction. <i>Journal of Organic Chemistry</i> , 2014, 79, 3094-3102.	3.2	26
23	Using the Source Function descriptor to dampen the multipole model bias in charge density studies from X-ray structure factors refinements. <i>Chemical Physics Letters</i> , 2009, 476, 308-316.	2.6	25
24	Atomistic Explanation for Interlayer Charge Transfer in Metal-Semiconductor Nanocomposites: The Case of Silver and Anatase. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5372-5377.	4.6	25
25	4-(1,2-diarylbut-1-en-1-yl)isobutyranilide derivatives as inhibitors of topoisomerase II. <i>European Journal of Medicinal Chemistry</i> , 2016, 118, 79-89.	5.5	24
26	Source Function applied to experimental densities reveals subtle electron-delocalization effects and appraises their transferability properties in crystals. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 180-193.	1.1	24
27	Structure-Activity Relationships of Hexahydrocyclopenta[<i>c</i>]quinoline Derivatives as Allosteric Inhibitors of CDK2 and EGFR. <i>ChemMedChem</i> , 2018, 13, 2627-2634.	3.2	23
28	Competing C=O...O, C=O...H...O, Cl...O, and Cl...Cl Interactions Governing the Structural Phase Transition of 2,6-Dichloro- <i>p</i> -benzoquinone at T _c = 122.6 K. <i>Crystal Growth and Design</i> , 2013, 13, 4571-4582.	3.0	22
29	Sequential Multicomponent Strategy for the Diastereoselective Synthesis of Densely Functionalized Spirooxindole-Fused Thiazolidines. <i>ACS Combinatorial Science</i> , 2018, 20, 98-105.	3.8	22
30	Probing an Allosteric Pocket of CDK2 with Small Molecules. <i>ChemMedChem</i> , 2017, 12, 33-41.	3.2	21
31	UV absorbing zwitterionic pyridinium-tetrazolate: exceptional transparency/optical nonlinearity trade-off. <i>Chemical Communications</i> , 2011, 47, 292-294.	4.1	20
32	Second Generation Nitrogen Doped Titania Nanoparticles: A Comprehensive Electronic and Microstructural Picture. <i>Chinese Journal of Chemistry</i> , 2014, 32, 1195-1213.	4.9	20
33	Model peptides containing the 3-sulfanyl-norbornene amino acid, a conformationally constrained cysteine analogue effective inducer of 3 ¹⁰ -helix secondary structures. <i>RSC Advances</i> , 2015, 5, 32643-32656.	3.6	20
34	Insights on spin polarization through the spin density source function. <i>Chemical Science</i> , 2015, 6, 3845-3852.	7.4	20
35	One step access to oxindole-based β -lactams through Ugi four-center three-component reaction. <i>RSC Advances</i> , 2018, 8, 34903-34910.	3.6	20
36	Spin Density Topology. <i>Molecules</i> , 2020, 25, 3537.	3.8	20

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37	Role of Pr on the Semiconductor Properties of Nanotitania. An Experimental and First-Principles Investigation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23083-23093.	3.1	19
38	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. <i>Tetrahedron</i> , 2002, 58, 5173-5178.	1.9	18
39	On the role of data quality in experimental charge-density studies. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2004, 60, 365-370.	0.3	18
40	Progress in the Understanding of the Key Pharmacophoric Features of the Antimalarial Drug Dihydroartemisinin: An Experimental and Theoretical Charge Density Study. <i>Chemistry - A European Journal</i> , 2013, 19, 3490-3503.	3.3	18
41	Crystallographic phase transitions in the $GdBaCo_2O_{7-x}$. <i>Physical Review B</i> , 2011, 84, .	3.2	17
42	Rationalizing the Lacking of Inversion Symmetry in a Noncentrosymmetric Polar Racemate: An Experimental and Theoretical Study. <i>Crystal Growth and Design</i> , 2014, 14, 5822-5833.	3.0	17
43	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. <i>Crystal Growth and Design</i> , 2016, 16, 6043-6054.	3.0	17
44	Molecular dynamics simulation of organic crystals: introducing the <i>CLP-dyncry</i> environment. <i>Journal of Applied Crystallography</i> , 2019, 52, 1253-1263.	4.5	17
45	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. <i>CrystEngComm</i> , 2020, 22, 7350-7360.	2.6	17
46	Charge ordering transition in $GdBaCo_2O_5$: Evidence of reentrant behavior. <i>Physical Review B</i> , 2013, 88, .	3.2	16
47	Rationalizing the Effect of Halogenation on the Molecular Structure of Simple Cyclobutene Derivatives by Topological Real-Space Analysis of Their Electron Density. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12695-12707.	2.5	15
48	Insights on spin delocalization and spin polarization mechanisms in crystals of azido copper(II) dinuclear complexes through the electron spin density Source Function. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 565-583.	1.1	14
49	Direct measurement and modeling of spontaneous charge migration across anataseâ€“brookite nanoheterojunctions. <i>Journal of Materials Chemistry A</i> , 2021, 9, 7782-7790.	10.3	14
50	Experimental and theoretical charge density distribution of the colossal magnetoresistive transition metal sulfide $FeCr_2S_4$. <i>Journal of Chemical Physics</i> , 2008, 128, 044710.	3.0	13
51	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. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3186-3196.	2.5	13
52	Conformational polymorphism in a Schiff-base macrocyclic organic ligand: an experimental and theoretical study. <i>Acta Crystallographica Section B: Structural Science</i> , 2010, 66, 527-543.	1.8	13
53	Synthesis of novel chiral β -isoxazoline derivatives related to ABT-418 and estimation of their affinity at neuronal nicotinic acetylcholine receptor subtypes. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 5594-5601.	5.5	13
54	Correlations of Crystal Structure and Solubility in Organic Salts: The Case of the Antiplasmodial Drug Piperazine. <i>Crystal Growth and Design</i> , 2019, 19, 1399-1410.	3.0	13

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55	Evading Pgp Activity in Drug-Resistant Cancer Cells: A Structural and Functional Study of Antitubulin Furan Metotica Compounds. <i>Molecular Cancer Therapeutics</i> , 2012, 11, 1103-1111.	4.1	12
56	Characterization of 2,4-Diamino-6-oxo-1,6-dihydropyrimidin-5-yl Ureido Based Inhibitors of <i>Trypanosoma brucei</i> FOLD and Testing for Antiparasitic Activity. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 7938-7948.	6.4	12
57	Anharmonic motions versus dynamic disorder at the Mg ion from the charge densities in pyrope (Mg ₃ Al ₂ Si ₃ O ₁₂) crystals at 30 K: six of one, half a dozen of the other. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 722-736.	1.1	12
58	Isonitrile-Based Multicomponent Synthesis of \hat{I}^2 -Amino Boronic Acids as \hat{I}^2 -Lactamase Inhibitors. <i>Antibiotics</i> , 2020, 9, 249.	3.7	12
59	Looking for structural phase transitions in the colossal magnetoresistive thiospinel FeCr ₂ S ₄ by a multi-temperature single-crystal X-ray diffraction study. <i>Chemical Physics Letters</i> , 2005, 416, 28-32.	2.6	11
60	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. <i>Crystal Growth and Design</i> , 2014, 14, 4418-4429.	3.0	11
61	Dynamic simulation of liquid molecular nanoclusters: structure, stability and quantification of internal (pseudo)symmetries. <i>New Journal of Chemistry</i> , 2019, 43, 2077-2084.	2.8	11
62	Enantio- and Regioselective Palladium(II)-Catalyzed Dioxygenation of (Aza)Alkenols. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 21723-21727.	13.8	11
63	Chemo- and Regioselective Palladium(II)-Catalyzed Aminoarylation of N-Allylureas Providing 4-Arylmethyl Imidazolidinones. <i>Synthesis</i> , 2019, 51, 3462-3470.	2.3	10
64	Switchable Oxidative Reactions of <i>N</i> -allyl-2-Aminophenols: Palladium-Catalyzed Alkoxyacyloxylation vs an Intramolecular Diels-Alder Reaction. <i>Organic Letters</i> , 2021, 23, 7698-7702.	4.6	10
65	Direct Synthesis of Fluorescent Oxazolo-phenoxazines by Copper-Catalyzed/Hypervalent Iodine(III)-Mediated Dimerization/Cyclization of 2-Benzylamino-phenols. <i>Journal of Organic Chemistry</i> , 2022, 87, 1032-1042.	3.2	10
66	Spin density accuracy and distribution in azido Cu(II) complexes: A source function analysis. <i>Journal of Computational Chemistry</i> , 2018, 39, 587-603.	3.3	9
67	Iodoamination of Alkenyl Sulfonamides by Potassium Iodide and Hydrogen Peroxide in Aqueous Medium. <i>Helvetica Chimica Acta</i> , 2019, 102, e1900088.	1.6	9
68	The fungal metabolite austdiol. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2003, 59, o199-o201.	0.4	8
69	A variable-temperature X-ray diffraction and theoretical study of conformational polymorphism in a complex organic molecule (DTC). <i>RSC Advances</i> , 2018, 8, 38445-38454.	3.6	8
70	Observation of an exotic lattice structure in the transparent $KTaO_3$ perovskite supercrystal. <i>Physical Review B</i> , 2020, 102, .	3.2	8
71	Molecular dynamics simulation of organic materials: structure, potentials and the MiCMoS computer platform. <i>CrystEngComm</i> , 2022, 24, 922-930.	2.6	8
72	Non-Decarboxylative Ruthenium-Catalyzed Rearrangement of 4-Alkylidene-isoxazol-5-ones to Pyrazole- and Isoxazole-4-carboxylic Acids. <i>Organic Letters</i> , 2022, , .	4.6	8

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73	Detection and kinetics of the single-crystal to single-crystal complete transformation of a thiiranium ion into thietanium ion. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7181.	2.8	7
74	Synthesis of unusual isoxazoline containing \hat{I}^2 and \hat{I}^3 -dipeptides as potential glutamate receptor ligands. <i>MedChemComm</i> , 2015, 6, 1260-1266.	3.4	7
75	On the molecular basis of the activity of the antimalarial drug chloroquine: EXAFS-assisted DFT evidence of a direct Fe \hat{I}^2 -N bond with free heme in solution. <i>Physica Scripta</i> , 2016, 91, 023001.	2.5	7
76	Molecular Dynamics Simulation of Molecular Crystals under Anisotropic Compression: Bulk and Directional Effects in Anthracene and Paracetamol. <i>Crystal Growth and Design</i> , 2020, 20, 7421-7428.	3.0	6
77	Design and synthesis of constrained bicyclic molecules as candidate inhibitors of influenza A neuraminidase. <i>PLoS ONE</i> , 2018, 13, e0193623.	2.5	6
78	Total Synthesis of (\hat{I}^2) \hat{I}^2 -Cannabidiol. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	2.4	6
79	The TACO Puzzle: A Phase-Transition Mystery Revisited. <i>Crystal Growth and Design</i> , 2018, 18, 7219-7227.	3.0	5
80	Stereodivergent Diversity \hat{I}^2 -Oriented Synthesis: Exploiting the Versatility of 2 \hat{I}^2 -Piperidine Ethanol. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 4013-4019.	2.4	5
81	Anharmonic Thermal Motion Modelling in the Experimental XRD Charge Density Determination of 1-Methyluracil at T = 23 K. <i>Molecules</i> , 2021, 26, 3075.	3.8	5
82	Kinetic-Bias Model for the Dynamic Simulation of Molecular Aggregation. The Liquid, Solute, Solvated-Nanodrop, and Solvated-Nanocrystal States of Benzoic Acid. <i>Crystal Growth and Design</i> , 2022, 22, 1857-1866.	3.0	5
83	Developing new \hat{I}^2 - and \hat{I}^2 -fructopyranose-based metal \hat{I}^2 -organic frameworks with nonlinear optical properties. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 210-218.	1.1	4
84	Highly diastereoselective entry to chiral oxindole-based \hat{I}^2 -amino boronic acids and spiro derivatives. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7211-7216.	2.8	4
85	Multi-temperature Electron Density Studies. , 2011, , 659-696.		3
86	Regioselective Preparation of Functionalized Isoxazoline Derivatives as Key Intermediates for the Synthesis of Selective N-Methyl-d-aspartate Receptor Antagonists. <i>Synthesis</i> , 2011, 2011, 1255-1260.	2.3	3
87	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
88	Synthesis of \hat{I}^2 -Tricholomic Acid Analogues and Pharmacological Characterization at Ionotropic Glutamate Receptors. <i>ChemistrySelect</i> , 2017, 2, 10295-10299.	1.5	3
89	Crystallization and structural properties of a family of isotopological 3D-networks: the case of a 4,4 \hat{I}^2 -bipy ligand \hat{I}^2 -M \hat{I}^2 + triflate system. <i>CrystEngComm</i> , 2018, 20, 3784-3795.	2.6	3
90	Allylation of isatin-derived N-Boc-hydrazones followed by Pd-catalyzed carboamination reaction: an entry to 3-spiro-pyrazolidyl-oxindoles. <i>RSC Advances</i> , 2019, 9, 37788-37800.	3.6	3

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91	Unravelling the Chemistry of the [Cu(4,7-Dichloroquinoline)2Br2]2 Dimeric Complex through Structural Analysis: A Borderline Ligand Field Case. <i>Crystals</i> , 2020, 10, 477.	2.2	3
92	Unexpected chiral vicinal tetrasubstituted diamines via borylcopper-mediated homocoupling of isatin imines. <i>Beilstein Journal of Organic Chemistry</i> , 2022, 18, 303-308.	2.2	3
93	A new monoclinic polymorph of 3-diethylamino-4-(4-methoxyphenyl)-1,1-dioxo-4H-1,2,4-triazete-4-carbonitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, o2032-o2033.	0.2	2
94	Crystal structure or chemical composition of salt-organic frameworks: what are the nonlinear optical properties due to?. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 506-514.	1.1	2
95	Enantio- and Regioselective Palladium(II)-Catalyzed Dioxygenation of (Z)-Alkenols. <i>Angewandte Chemie</i> , 2021, 133, 21891-21895.	2.0	2
96	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. <i>Crystals</i> , 2020, 10, 894.	2.2	1
97	Insights on spin-polarization via the spin density Source Function. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, C281-C281.	0.1	1
98	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.. <i>ChemInform</i> , 2002, 33, 50-50.	0.0	0
99	Insights on spin-density delocalization/polarization mechanisms through the source function. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C1434-C1434.	0.1	0
100	Phase Stability and Morphology of Gel Grown Crystals: The Case of CdCl2-bpp Polymeric System. <i>Crystals</i> , 2019, 9, 363.	2.2	0
101	Decoding conformational polymorphism in organic substances. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, C557-C557.	0.1	0
102	CLPdyn: a cheap and reliable tool for molecular dynamics studies of organic molecules in the condensed phase. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, e540-e540.	0.1	0