

Stefano Leoni

List of Publications by Year in descending order

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120
papers

2,763
citations

172207

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128
docs citations

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times ranked

3892
citing authors

#	ARTICLE	IF	CITATIONS
1	Product tunable behavior of carbon nanotubes-supported Ni ^{II} -Fe catalysts for guaiacol hydrodeoxygenation. <i>Applied Catalysis A: General</i> , 2017, 529, 20-31.	2.2	153
2	Route to a Family of Robust, Non-Interpenetrated Metal-Organic Frameworks with p6mm-like Topology. <i>Chemistry - A European Journal</i> , 2011, 17, 13007-13016.	1.7	127
3	Enumeration of Not-Yet-Synthesized Zeolitic Zinc Imidazolate MOF Networks: A Topological and DFT Approach. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9437-9443.	1.2	93
4	Superhard allotropes with odd and even ring topologies. <i>Physical Review B</i> , 2011, 84, .	1.1	91
5	Understanding the nature of "superhard graphite". <i>Scientific Reports</i> , 2012, 2, 471.	1.6	86
6	Squeezing lone pairs: The 17 to 7 pressure-induced phase transition in black phosphorus. <i>Physical Review B</i> , 2012, 85, .	1.1	81
7	Nucleation and Growth in Pressure-Induced Phase Transitions from Molecular Dynamics Simulations: Mechanism of the Reconstructive Transformation of NaCl to the CsCl-Type Structure. <i>Physical Review Letters</i> , 2004, 92, 250201.	2.9	79
8	Packings of Carbon Nanotubes - New Materials for Hydrogen Storage. <i>Advanced Materials</i> , 2011, 23, 1237-1241.	11.1	76
9	Normal-state correlated electronic structure of iron pnictides from first principles. <i>Physical Review B</i> , 2008, 78, .	1.1	73
10	Hydrogen Adsorption Sites in Zeolite Imidazolate Frameworks ZIF-8 and ZIF-11. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13381-13384.	1.5	66
11	On the Mechanism of Gold/NHC Compounds Binding to DNA G-Quadruplexes: Combined Metadynamics and Biophysical Methods. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 14524-14528.	7.2	60
12	Mechanism of the pressure-induced wurtzite to rocksalt transition of CdSe. <i>Physical Review B</i> , 2005, 72, .	1.1	52
13	Zeolitic imidazolate framework-71 nanocrystals and a novel SOD-type polymorph: solution mediated phase transformations, phase selection via coordination modulation and a density functional theory derived energy landscape. <i>Dalton Transactions</i> , 2014, 43, 3528.	1.6	52
14	The mechanism of aquaporin inhibition by gold compounds elucidated by biophysical and computational methods. <i>Chemical Communications</i> , 2017, 53, 3830-3833.	2.2	50
15	Ce ₄ [Si ₄ O ₄ N ₆]O-A Hyperbolically Layered Oxonitridosilicate Oxide with an Ordered Distribution of Oxygen and Nitrogen. <i>Chemistry - A European Journal</i> , 2000, 6, 2714-2720.	1.7	47
16	High-pressure crystal chemistry of binary intermetallic compounds. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2006, 221, 420-434.	0.4	46
17	Walking the Path from B ₄ - to B ₁ -Type Structures in GaN. <i>Physical Review Letters</i> , 2007, 99, 125505.	2.9	46
18	A two-electron mechanism of lithium insertion into layered Li_xMoO_3 : a DFT and DFT+U study. <i>Journal of Materials Chemistry A</i> , 2013, 1, 1778-1784.	5.2	46

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19	Structure and Reactivity of $[\text{Mo}_3\text{S}_4\text{S}_2]^{4+}$ Complexes. Quantum Chemical Calculations, X-ray Structural Characterization, and Raman Spectroscopic Measurements. <i>Inorganic Chemistry</i> , 1998, 37, 2633-2644.	1.9	45
20	Atomistic investigation of Li ⁺ diffusion pathways in the olivine LiFePO ₄ cathode material. <i>Journal of Materials Chemistry</i> , 2011, 21, 16365.	6.7	42
21	Insulator-metal transition in the doped 3d transition metal oxide LaTiO ₃ . <i>Physical Review B</i> , 2004, 70, .	1.1	38
22	Hydrogen storage in zeolite imidazolate frameworks. A multiscale theoretical investigation. <i>International Journal of Hydrogen Energy</i> , 2011, 36, 6005-6013.	3.8	38
23	Subtle polymorphism of zinc imidazolate frameworks: temperature-dependent ground states in the energy landscape revealed by experiment and theory. <i>CrystEngComm</i> , 2013, 15, 4036-4040.	1.3	38
24	Structural tuning and catalysis of tungsten carbides for the regioselective cleavage of C-O bonds. <i>Journal of Catalysis</i> , 2019, 369, 283-295.	3.1	38
25	Competing intermediates in the pressure-induced wurtzite to rocksalt phase transition in ZnO. <i>Physical Review B</i> , 2008, 78, .	1.1	33
26	On Tilings and Patterns on Hyperbolic Surfaces and Their Relation to Structural Chemistry. <i>ChemPhysChem</i> , 2001, 2, 413-422.	1.0	31
27	Modelling of the $\hat{\Gamma}_8$ (clathrate VIII) \leftrightarrow $\hat{\Gamma}_2$ (clathrate I) phase transition in Eu ₈ Ga ₁₆ Ge ₃₀ . <i>Journal of Alloys and Compounds</i> , 2003, 350, 113-122.	2.8	31
28	Novel metastable metallic and semiconducting germaniums. <i>Scientific Reports</i> , 2013, 3, 1466.	1.6	31
29	Low-dimensional sublattice melting by pressure: Superionic conduction in the phase interfaces of the fluorite-to-cotunnite transition of CaF ₂ . <i>Physical Review B</i> , 2006, 74, .	1.1	30
30	Molecular Basis of Aquaporin-7 Permeability Regulation by pH. <i>Cells</i> , 2018, 7, 207.	1.8	30
31	Electrodynamic response of incoherent metals: Normal phase of iron pnictides. <i>Physical Review B</i> , 2009, 79, .	1.1	29
32	Unconventional Mott transition in $\text{K}_2\text{Fe}_2\text{Se}_2$. <i>Physical Review B</i> , 2011, 84, .	1.1	29
33	The energy landscapes of zeolitic imidazolate frameworks (ZIFs): towards quantifying the presence of substituents on the imidazole ring. <i>Journal of Materials Chemistry</i> , 2012, 22, 10152-10154.	6.7	29
34	Putting the squeeze on NaCl: modelling and simulation of the pressure driven B1-B2 phase transition. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2004, 219, 339-344.	0.4	28
35	Nanodomain fragmentation and local rearrangements in CdSe under pressure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 19612-19616.	3.3	27
36	Microwave-Assisted Synthesis of Defects Metal-Imidazolate-Amide-Imidate Frameworks and Improved CO ₂ Capture. <i>Inorganic Chemistry</i> , 2015, 54, 10073-10080.	1.9	27

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37	Comparative study of tetragonal and hexagonal FeSe: An orbital-selective scenario. Europhysics Letters, 2010, 92, 67003.	0.7	26
38	An Isorecticular Family of Microporous Metal-Organic Frameworks Based on Zinc and 2-Substituted Imidazolate-4,5-Imidate: Syntheses, Structures and Properties. Chemistry - A European Journal, 2012, 18, 11630-11640.	1.7	26
39	A zeolitic imidazolate framework with conformational variety: conformational polymorphs versus frameworks with static conformational disorder. CrystEngComm, 2016, 18, 2477-2489.	1.3	26
40	Orbital-spin order and the origin of structural distortion in $MgTi_{2-x}Mn_x$. Physical Review B, 2008, 78, .	1.1	25
41	Modelling polymorphs of metal-organic frameworks: a systematic study of diamondoid zinc imidazolates. CrystEngComm, 2010, 12, 2809.	1.3	25
42	Mechanism of Germacradien-4-ol Synthase-Controlled Water Capture. Biochemistry, 2016, 55, 2112-2121.	1.2	25
43	Dynamic Displacement Disorder of Cubic $BaTiO_3$. Physical Review Letters, 2018, 120, 167601.	2.9	25
44	$Zn_3(C_6H_{14}N_2)_3[B_6P_{12}O_{39}(OH)_{12}] \cdot \epsilon\text{-}\epsilon\text{-}(C_6H_{14}N_2)[HPO_4]$: A Chiral Borophosphate - Triethylenediammonium Hydrogenphosphate Composite. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2002, 628, 67-76.	0.6	24
45	Multicenter multidomain $B_1 \sim B_2$ pressure-induced reconstructive phase transition in potassium fluoride. Physical Review B, 2005, 72, .	1.1	23
46	Polymorphs of lithium-boron imidazolates: energy landscape and hydrogen storage properties. Dalton Transactions, 2011, 40, 3796-3798.	1.6	22
47	Formation, Structure, and Polymorphism of Novel Lowest-Dimensional AgI Nanoaggregates by Encapsulation in Carbon Nanotubes. Small, 2007, 3, 1730-1734.	5.2	21
48	$BaAl_2Ge_2$: synthesis, crystal structure, magnetic and electronic properties, chemical bonding, and atomistic model of the $I \pm \hat{t}^2$ phase transition. Solid State Sciences, 2003, 5, 139-148.	1.5	20
49	Atomistic modeling of diffuse scattering in cubic $PbZrO_3$. Phase Transitions, 2015, 88, 273-282.	0.6	20
50	Aquaporin-driven hydrogen peroxide transport: a case of molecular mimicry?. RSC Chemical Biology, 2020, 1, 390-394.	2.0	20
51	Low-temperature metal-insulator transition in the electron-doped iron chalcogenide FeSe superconductor. Europhysics Letters, 2010, 91, 27001.	0.7	19
52	Unveiling the Mechanisms of Aquaglyceroporin-3 Water and Glycerol Permeation by Metadynamics. Chemistry - A European Journal, 2019, 25, 8713-8718.	1.7	19
53	Local structure in the paraelectric phase of $Cd_{1-x}Mn_x$ from x-ray diffuse scattering, by means of <i>ab initio</i> molecular dynamics and Monte Carlo modeling. Physical Review B, 2010, 81, .	1.1	18
54	$\hat{I}^2Ca_3N_2$, a Metastable Nitride in the System $Ca \sim N$. Chemistry - A European Journal, 2009, 15, 3419-3425.	1.7	17

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55	Polarized Cluster Dynamics at the Paraelectric to Ferroelectric Phase Transition in BaTiO ₃ . Journal of Physical Chemistry B, 2010, 114, 16465-16470.	1.2	17
56	Hierarchical thermoelectrics: crystal grain boundaries as scalable phonon scatterers. Nanoscale, 2016, 8, 3729-3738.	2.8	17
57	Solidâ€“Solid Phase Transitions: Interface Controlled Reactivity and Formation of Intermediate Structures. Chemistry - A European Journal, 2007, 13, 10022-10029.	1.7	16
58	Microscopic description of insulator-metal transition in high-pressure oxygen. Scientific Reports, 2017, 7, 2632.	1.6	16
59	Templated Chromophore Assembly on Peptide Scaffolds: A Structural Evolution. Chemistry - A European Journal, 2018, 24, 16136-16148.	1.7	16
60	On the Mechanism of Gold/NHC Compounds Binding to DNA Gâ€“Quadruplexes: Combined Metadynamics and Biophysical Methods. Angewandte Chemie, 2018, 130, 14732-14736.	1.6	16
61	Li ₃ [ScN ₂]: The First Nitridoscandate(III)â€“Tetrahedral Sc Coordination and Unusual MX ₂ Framework. Chemistry - A European Journal, 2003, 9, 4255-4259.	1.7	15
62	Ae[Be ₂ N ₂]: Nitridoberyllates of the Heavier Alkaline-Earth Metals. Angewandte Chemie - International Edition, 2004, 43, 1088-1092.	7.2	15
63	Mechanisms and Nucleation Characteristics of the Pressure-Induced B1â€“B2 Transition in Potassium Halides: A Question of Ion Hardness and Softness. Journal of Physical Chemistry B, 2006, 110, 10873-10877.	1.2	15
64	Tunable Kondo-Mott physics in bulk Bi ₂ Te ₃ topological insulator. Physical Review B, 2012, 85, .	1.1	14
65	Novel Barium Beryllates Ba[Be ₂ N ₂] and Ba ₃ [Be ₅ O ₈]: Syntheses, Crystal Structures and Bonding Properties. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1818-1824.	0.6	13
66	Bulk quantum correlations and doping-induced nonmetallicity in the Bi ₂ Se ₃ topological insulator. Physical Review B, 2012, 85, .	1.1	13
67	Theoretical investigation of the electronic structure and quantum transport in the grapheneâ€“C(111) diamond surface system. Journal of Physics Condensed Matter, 2013, 25, 435302.	0.7	13
68	Kondoesque origin of resistivity anisotropy in graphite. Physical Review B, 2013, 87, .	1.1	13
69	Magnetoresistance in the Spin-Orbit Kondo State of Elemental Bismuth. Scientific Reports, 2015, 5, 13772.	1.6	13
70	Selective orbital reconstruction in tetragonal FeS: A density functional dynamical mean-field theory study. Scientific Reports, 2017, 7, 46439.	1.6	13
71	Mechanism of the pressure induced reconstructive transformation of KCl from the NaCl type to the CsCl type structure. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, .	0.4	12
72	VNb ₉ O ₂₅ â€“Synthesis, electrical conducting behaviour and density functional theory (DFT) calculation. Journal of Solid State Chemistry, 2009, 182, 2053-2060.	1.4	12

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73	Electrodynamics and quantum capacity of Li_xFePO_4 battery material. Applied Physics Letters, 2011, 99, 192103.	1.5	12
74	Indium Imidazolate Frameworks with Differently Distorted ReO_3 -Type Structures: Syntheses, Structures, Phase Transitions, and Crystallization Studies. Crystal Growth and Design, 2014, 14, 4664-4673.	1.4	11
75	The role of covalency in the orbital-order of 3d1 perovskites. Solid State Sciences, 2006, 8, 1138-1143.	1.5	10
76	Hidden orbital fluctuations in the solid solution $\text{Y}_{1-x}\text{La}_x\text{TiO}_3$ ($x < 0.2$). Physical Review B, 2006, 74, .	1.1	10
77	Extending the scope of "in silico experiments": Theoretical approaches for the investigation of reaction mechanisms, nucleation events and phase transitions. Science and Technology of Advanced Materials, 2007, 8, 434-441.	2.8	10
78	Self-doping induced orbital-selective Mott transition in $\text{Hg}_2\text{Ru}_2\text{O}_7$. Physical Review B, 2009, 79, .	1.1	10
79	Orbital-selective Mottness in layered iron oxychalcogenides: the case of $\text{Na}_2\text{Fe}_2\text{OSe}_2$. Journal of Physics Condensed Matter, 2014, 26, 145602.	0.7	9
80	Metastable metal imidazolates: development of targeted syntheses by combining experimental and theoretical investigations of the formation mechanisms. Zeitschrift Fur Kristallographie - Crystalline Materials, 2014, 229, 807-822.	0.4	9
81	Pressure-induced orbital-selective metal from the Mott insulator BaFe_2As_2 . Physical Review B, 2020, 101, 080401.		
82	Orbital-selective charge dynamics in YTiO_3 across the magnetic transition: Combined local-density approximation and dynamical mean-field theory. Physical Review B, 2007, 76, 080401.	1.1	8
83	Theory of the orbital-selective Mott transition in ferromagnetic YTiO_3 under high pressure. Physical Review B, 2008, 77, 080401.	1.1	7
84	The ZIF system zinc(II) 4,5-dichoroimidazolate: theoretical and experimental investigations of the polymorphism and crystallization mechanisms. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 77-90.	0.4	7
85	Electron localization in olivine materials for advanced lithium-ion batteries. Journal of Applied Physics, 2012, 111, 112602.	1.1	6
86	Enzymatic synthesis of natural (+)-aristolochene from a non-natural substrate. Chemical Communications, 2016, 52, 14027-14030.	2.2	6
87	Novel Carbons: Habits and Oddities. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2014, 640, 681-688.	0.6	5
88	Metashooting: a novel tool for free energy reconstruction from polymorphic phase transition mechanisms. Faraday Discussions, 2018, 211, 235-251.	1.6	5
89	Elucidation of simple pathways for reconstructive phase transitions using periodic equi-surfaces (PES) descriptors. II. The strontium disilicide transition. Solid State Sciences, 2003, 5, 95-107.	1.5	4
90	Chemical, thermal, and theoretical analysis of the Ba_3Tt_4 phase transition of Ba_3Tt_4 compounds. Zeitschrift Fur Kristallographie - Crystalline Materials, 2003, 218, 171-177.	0.4	4

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91	Atomistic engineering in the control of the electronic properties of CdSe nanotubes. Physical Review B, 2010, 82, .	1.1	4
92	Materials for Lithium Ion Batteries: Challenges for Numerical Simulations. Zeitschrift Fur Physikalische Chemie, 2012, 226, 95-106.	1.4	4
93	Mechanisms of irreversible aquaporin-10 inhibition by organogold compounds studied by combined biophysical methods and atomistic simulations. Metallomics, 2021, 13, .	1.0	4
94	On the continuous transformations between genus-3 minimal surfaces approximants. Zeitschrift Für Kristallographie, 2011, 226, 678-683.	1.1	3
95	A Walk on the Chemical Landscape: The Role of B33 along the B1â€“B2 Phase Transition in RbF and NaBr. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 864-869.	0.6	3
96	Framework reconstruction between hR8 and cI16 germaniums: A molecular dynamics study. RSC Advances, 2012, 2, 8833.	1.7	3
97	GerÃ¼stverbindungen mit beweglichen LaIII-Kationen: Synthesen, Kristallstrukturen und Strukturodynamik der Lanthan(III)-Eisen(II)-Sulfid-Halogenide La53Fe12S90X3 (X = Cl, Br, I). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 107-114.	0.6	2
98	Subtle Polymorphism in the Zinc Imidazolate System. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 2086-2086.	0.6	2
99	On Tilings and Patterns on Hyperbolic Surfaces and Their Relation to Structural Chemistry. , 2001, 2, 413.		2
100	PbTe/PbSe Thermoelectric Nanocomposites: The Impact of Length Modulations on Lowering Thermal Conductivity. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , .	0.6	2
101	Deconstructing Sodalite with Hyperbolic Tilings: A PNS Approach. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 619-623.	0.6	1
102	All-t2g Electronic Orbital Reconstruction of Monoclinic MoO2 Battery Material. Applied Sciences (Switzerland), 2020, 10, 5730.	1.3	1
103	Pressure-induced structural transformation of clathrate $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{Ge} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 136 \langle \text{mml:mdiv} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{ via ultrafast recrystallization of an amorphous intermediate. Physical Review B, 2022, 105, .$		
104	Modelling of the \hat{I}_{\pm} (Clathrate VIII) $\hat{I}_{\pm} \hat{I}_{\pm}^2$ (Clathrate I) Phase Transition in Eu8Ga16Ge30.. ChemInform, 2003, 34, no.	0.1	0
105	BaAl2Ge2: Synthesis, Crystal Structure, Magnetic and Electronic Properties, Chemical Bonding, and Atomistic Model of the $\hat{I}_{\pm} \hat{I}_{\pm}^2$ Phase Transition.. ChemInform, 2003, 34, no.	0.1	0
106	Li3[ScN2]: The First Nitridoscandate(III)â€”Tetrahedral Sc Coordination and Unusual MX2 Framework.. ChemInform, 2003, 34, no.	0.1	0
107	Ae[Be2N2]: Nitridoberyllates of the Heavier Alkaline-Earth Metals.. ChemInform, 2004, 35, no.	0.1	0
108	Novel Barium Beryllates Ba[Be2N2] and Ba3[Be5O8]: Syntheses, Crystal Structures and Bonding Properties.. ChemInform, 2005, 36, no.	0.1	0

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109	Full-Featured Simulation of Reconstructive Solid-Solid Phase Transitions. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 2086-2086.	0.6	0
110	Publisher's Note: Low-dimensional sublattice melting by pressure: Superionic conduction in the phase interfaces of the fluorite-to-cotunnite transition of CaF ₂ [Phys. Rev. B74, 094106 (2006)]. Physical Review B, 2006, 74, .	1.1	0
111	Microscopic Mechanism and Domain Formation in the Paraelectric to Ferroelectric Phase Transitions in BaTiO ₃ . Materials Research Society Symposia Proceedings, 2007, 1034, 84.	0.1	0
112	The Role of Interfaces in Ionic Conductors and Ferroelectrics. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 2013-2013.	0.6	0
113	Structural transitions in solids. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 505-506.	0.3	0
114	Novel Computational Approaches to Li Diffusion and Electron Transport for High Capacity Battery Materials. Materials Research Society Symposia Proceedings, 2011, 1313, 70101.	0.1	0
115	Redesign of Carbon Materials for Novel Storage, Mechanical and Optical Properties. Materials Research Society Symposia Proceedings, 2012, 1451, 9-14.	0.1	0
116	Materials for Lithium Ion Batteries: Challenges for Numerical Simulations. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1555-1555.	0.6	0
117	Reticular Materials for Hydrogen Storage. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1626-1626.	0.6	0
118	Redesign of Carbon Materials for Novel Storage, Mechanical and Optical Properties. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1626-1626.	0.6	0
119	The rules of metastability: detailed transformation mechanisms in chemical elements by means of molecular dynamics techniques. Chemical Modelling, 2014, , 30-56.	0.2	0
120	Harvesting Free Energy Landscapes in Biological Systems. Lecture Notes in Bioengineering, 2020, , 64-77.	0.3	0