Alessandro Stroppa

List of Publications by Year
in descending order

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118 papers	7,171 citations	57631 44 h-index	56606 83 g-index
123 all docs	123 docs citations	123 times ranked	8300 citing authors

#	Article	IF	Citations
1	Hybrid functionals applied to extended systems. Journal of Physics Condensed Matter, 2008, 20, 064201.	0.7	500
2	Accurate surface and adsorption energies from many-body perturbation theory. Nature Materials, 2010, 9, 741-744.	13.3	476
3	Hybrid Improper Ferroelectricity in a Multiferroic and Magnetoelectric Metalâ€Organic Framework. Advanced Materials, 2013, 25, 2284-2290.	11.1	280
4	Tuning the Ferroelectric Polarization in a Multiferroic Metalâ€“Organic Framework. Journal of the American Chemical Society, 2013, 135, 18126-18130.	6.6	252
5	Electric Control of Magnetization and Interplay between Orbital Ordering and Ferroelectricity in a Multiferroic Metalâ€“Organic Framework. Angewandte Chemie - International Edition, 2011, 50, 5847-5850.	7.2	249
6	Tunable ferroelectric polarization and its interplay with spinâ€“orbit coupling in tin iodide perovskites. Nature Communications, 2014, 5, 5900.	5.8	247
7	Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites. Scientific Reports, 2016, 6, 28618.	1.6	234
8	Intrinsic and anisotropic Rashba spin splitting in Janus transition-metal dichalcogenide monolayers. Physical Review B, 2018, 97, .	1.1	228
9	The shortcomings of semi-local and hybrid functionals: what we can learn from surface science studies. New Journal of Physics, 2008, 10, 063020.	1.2	222
10	Electronic structure and ferromagnetism of Mn-doped group-IV semiconductors. Physical Review B, 2003, 68, .	1.1	195
11	Ferroelectric Polarization of CH₃NH₃PbI₃: A Detailed Study Based on Density Functional Theory and Symmetry Mode Analysis. Journal of Physical Chemistry Letters, 2015, 6, 2223-2231.	2.1	179
12	Cross coupling between electric and magnetic orders in a multiferroic metal-organic framework. Scientific Reports, 2014, 4, 6062.	1.6	175
13	Hybrid functional study of proper and improper multiferroics. Physical Chemistry Chemical Physics, 2010, 12, 5405.	1.3	147
14	Spin-phonon coupling effects in transition-metal perovskites: A DFTÂ+Â<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>and hybrid-functional study. Physical Review B, 2012, 85, .	1.1	145
15	CO adsorption on metal surfaces: A hybrid functional study with plane-wave basis set. Physical Review B, 2007, 76, .	1.1	133
16	Emergence of ferroelectricity and spin-valley properties in two-dimensional honeycomb binary compounds. Physical Review B, 2015, 91, .	1.1	128
17	Unraveling the Jahn-Teller effect in Mn-doped GaN using the Heyd-Scuseria-Ernzerhof hybrid functional. Physical Review B, 2009, 79, .	1.1	122
18	Magnetism in C- or N-doped MgO and ZnO: A Density-Functional Study of Impurity Pairs. Physical Review Letters, 2010, 105, 267203.	2.9	111

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19	Switchable electric polarization and ferroelectric domains in a metal-organic-framework. Npj Quantum Materials, 2016, 1, .	1.8	103
20	Experimental and theoretical studies of structural phase transition in a novel polar perovskite-like [C₂H₅NH₃][Na_{0.5}Fe_{0.5}(HCOO)₃] formate. Dalton Transactions, 2016, 45, 2574-2583.	1.6	103
21	The multiferroic phase of DyFeO₃: anab initiostudy. New Journal of Physics, 2010, 12, 093026.	1.2	100
22	Multiferroicity in TTF-CA Organic Molecular Crystals Predicted throughAbÂInitioCalculations. Physical Review Letters, 2009, 103, 266401.	2.9	94
23	Large ferroelectric polarization in the new double perovskite NaLaMnWO6 induced by non-polar instabilities. Physical Chemistry Chemical Physics, 2011, 13, 12186.	1.3	93
24	Possibility of combining ferroelectricity and Rashba-like spin splitting in monolayers of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi></mml:mrow></mml:m transition-metal dichalcogenides<mml:math		

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37	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. Journal of Physical Chemistry C, 2017, 121, 23045-23054.	1.5	56
38	Coexistence of Three Ferroic Orders in the Multiferroic Compound [(CH₃)₄N][Mn(N₃)₃] with Perovskiteâ€Like Structure. Chemistry - A European Journal, 2016, 22, 7863-7870.	1.7	54
39	Lone-Pair-Electron-Driven Ionic Displacements in a Ferroelectric Metalâ€“Organic Hybrid. Inorganic Chemistry, 2016, 55, 10337-10342.	1.9	51
40	Revealing the role of thiocyanate anion in layered hybrid halide perovskite (CH3NH3)2Pb(SCN)2I2. Journal of Chemical Physics, 2017, 146, 224702.	1.2	49
41	Electric-Magneto-Optical Kerr Effect in a Hybrid Organicâ€“Inorganic Perovskite. Journal of the American Chemical Society, 2017, 139, 12883-12886.	6.6	49
42	Origin of Ferroelectricity in Two Prototypical Hybrid Organicâ€“Inorganic Perovskites. Journal of the American Chemical Society, 2022, 144, 816-823.	6.6	47
43	Magnetic phase transition and giant anisotropic magnetic entropy change in TbFeO3 single crystal. Journal of Applied Physics, 2016, 119, .	1.1	46
44	Spin-reorientation magnetic transitions in Mn-doped SmFeO₃. IUCrJ, 2017, 4, 598-603.	1.0	46
45	Polar distortions in hydrogen-bonded organic ferroelectrics. Physical Review B, 2011, 84, .	1.1	45
46	Intertwined Rashba, Dirac, and Weyl Fermions in Hexagonal Hyperferroelectrics. Physical Review Letters, 2016, 117, 076401.	2.9	42
47	Adsorption and Dissociation of CO on Bare and Ni-Decorated Stepped Rh(553) Surfaces. Journal of Physical Chemistry C, 2009, 113, 942-949.	1.5	39
48	Structural, electronic and ferroelectric properties of croconic acid crystal: a DFT study. Physical Chemistry Chemical Physics, 2012, 14, 14673.	1.3	39
49	Ferroelectric polarization of hydroxyapatite from density functional theory. RSC Advances, 2017, 7, 21375-21379.	1.7	37
50	Ferroelectricity and ferromagnetism in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>VO</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> monolayer: Role of the Dzyaloshinskii-Moriya interaction. Physical Review B, 2020, 102, .	1.1	37
51	Exceptionally large room-temperature ferroelectric polarization in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">PbNiO</mml:mi><mml:mn mathvariant="bold">3</mml:mn></mml:msub></mml:math>multiferroic nickelate: First-principles study. Physical Review B, 2012, 86, .	1.1	36
52	Brilliant triboluminescence in a potential organicâ€“inorganic hybrid ferroelectric: (Ph₃PO)₂MnBr₂. Inorganic Chemistry Frontiers, 2017, 4, 154-159.	3.0	36
53	Advances in ab-initio theory of multiferroics. European Physical Journal B, 2012, 85, 1.	0.6	35
54	Persistent Spin-texture and Ferroelectric Polarization in 2D Hybrid Perovskite Benzylammonium Lead-halide. Journal of Physical Chemistry Letters, 2020, 11, 5177-5183.	2.1	34

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55	Computational and experimental imaging of Mn defects on GaAs (110) cross-sectional surfaces. Physical Review B, 2007, 75, .	1.1	33
56	Competing magnetic phases of Mn5Ge3compound. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 44-52.	0.8	33
57	Magnetic Structures of Heterometallic M(II)â€“M(III) Formate Compounds. Inorganic Chemistry, 2017, 56, 197-207.	1.9	33
58	Bioferroelectric Properties of Glycine Crystals. Journal of Physical Chemistry Letters, 2019, 10, 1319-1324.	2.1	32
59	Magneto-Optical Kerr Switching Properties of (CrI₃)₂ and (CrBr₃/CrI₃) Bilayers. ACS Applied Electronic Materials, 2020, 2, 1373-1380.	2.0	32
60	Tuning the Weak Ferromagnetic States in Dysprosium Orthoferrite. Scientific Reports, 2016, 6, 37529.	1.6	31
61	A RAIRS, TPD, and DFT Study of Carbon Monoxide Adsorption on Stepped Rh(553). Journal of Physical Chemistry C, 2008, 112, 806-812.	1.5	30
62	Composition and strain dependence of band offsets at metamorphicInxGa1â^'xAsâ•InyAl1â^'yAsheterostructures. Physical Review B, 2005, 71, .	1.1	29
63	Tuning the ferroelectric polarization in AAâ€²MnWO₆ double perovskites through A cation substitution. Dalton Transactions, 2015, 44, 10644-10653.	1.6	29
64	Lattice dynamics of Dirac node-line semimetal ZrSiS. Physical Review B, 2017, 96, .	1.1	28
65	Fingerprints of the hydrogen bond in the photoemission spectra of croconic acid condensed phase: An x-ray photoelectron spectroscopy and ab-initio study. Journal of Chemical Physics, 2011, 134, 174505.	1.2	26
66	Switchable Rashba anisotropy in layered hybrid organicâ€“inorganic perovskite by hybrid improper ferroelectricity. Npj Computational Materials, 2020, 6, .	3.5	26
67	Cyano-bridged perovskite [(CH3)3NOH]2[KM(CN)6], [M: Fe(iii), and Co(iii)] for high-temperature multi-axial ferroelectric applications with enhanced thermal and nonlinear optical performance. Journal of Materials Chemistry C, 2020, 8, 17491-17501.	2.7	26
68	Magneto-optical properties of (Ga,Mn)As: Anab initiodetermination. Physical Review B, 2008, 77, .	1.1	24
69	The electronic structure of gas phase croconic acid compared to the condensed phase: More insight into the hydrogen bond interaction. Journal of Chemical Physics, 2013, 138, 014308.	1.2	24
70	Atomically precise semiconductorâ€”graphene and hBN interfaces by Ge intercalation. Scientific Reports, 2015, 5, 17700.	1.6	24
71	Improper ferroelectricity at antiferromagnetic domain walls of perovskite oxides. Physical Review B, 2017, 96, .	1.1	24
72	Structural and ferroelectric transitions in magnetic nickelate PbNiO₃. New Journal of Physics, 2014, 16, 015030.	1.2	23

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73	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	1.9	23
74	On The Density Functional Theory Treatment of Lanthanide Coordination Compounds: A Comparative Study in a Series of Cuâ€“Ln (Ln = Gd, Tb, Lu) Binuclear Complexes. Inorganic Chemistry, 2017, 56, 9474-9485.	1.9	22
75	Tunable spin textures in polar antiferromagnetic hybrid organicâ€“inorganic perovskites by electric and magnetic fields. Npj Computational Materials, 2020, 6, .	3.5	22
76	Ab initiostudy of the relation between electric polarization and electric field gradients in ferroelectrics. Physical Review B, 2012, 86, .	1.1	20
77	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. Physical Review Materials, 2019, 3, .	0.9	20
78	Electronic structure of tris(8-hydroxyquinolinato)aluminium(III) revisited using the Heyd-Scuseria-Ernzerhof hybrid functional: Theory and experiments. Physical Review B, 2011, 84, .	1.1	17
79	Tuning order-by-disorder multiferroicity in CuO by doping. Physical Review B, 2014, 90, .	1.1	17
80	Spin polarization tuning in Mn5â^'xFexGe3. Applied Physics Letters, 2008, 93, 092502.	1.5	16
81	Electronic transport of organic-inorganic hybrid perovskites from first-principles and machine learning. Applied Physics Letters, 2019, 114, .	1.5	16
82	Polar and Magneto-Electric Properties of Anti-Ferrodistortive Ordered Jahn-Teller Distortions in a multiferroic metal-organic framework. Journal of Physics: Conference Series, 2013, 428, 012029.	0.3	15
83	Structural and magnetic properties of Mn-doped GaAs(1â€‰1â€‰0) surface. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2006, 126, 217-221.	1.7	14
84	Kinetic asymmetry in the growth of two-dimensional Mn oxide nanostripes. Physical Review B, 2013, 88, .	1.1	14
85	Structural properties and strain engineering of a BeB₂ monolayer from first-principles. RSC Advances, 2017, 7, 38410-38414.	1.7	14
86	Two-dimensional metal dicyanamide frameworks of BeTriMe[M(dca)3(H2O)] (BeTriMe =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 232 Td (magnetic orders and nonlinear optical threshold temperature sensing. Journal of Materials Chemistry C, 2020, 8, 11735-11747.	2.7	14
87	ZnSeâ^•GaAs(001)heterostructures with defected interfaces: Structural, thermodynamic, and electronic properties. Physical Review B, 2005, 72, .	1.1	13
88	Magneto-electric coupling in antiferromagnet/ferroelectric Mn2Au/BaTiO3 interface. Journal of Applied Physics, 2016, 120, .	1.1	12
89	Noble gas endohedral fullerenes, Ng@C60 (Ng=Ar, Kr): a particular benchmark for assessing the account of non-covalent interactions by density functional theory calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	11
90	Cubic and tetragonal perovskites from the random phase approximation. Physical Review Materials, 2019, 3, .	0.9	10

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91	Tuning the CO Dissociation Barriers by Low-Dimensional Surface Alloys. Journal of Physical Chemistry C, 2011, 115, 21320-21323.	1.5	9
92	Pressure-induced reversible framework rearrangement and increased polarization in the polar [NH4][Cd(HCOO)3] hybrid perovskite. Inorganic Chemistry Frontiers, 2019, 6, 2379-2386.	3.0	9
93	Non-collinear magnetic states of Mn5Ge3 compound. Materials Science in Semiconductor Processing, 2006, 9, 841-847.	1.9	8
94	Synthesis and Characterization of MnCrO4, a New Mixed-Valence Antiferromagnet. Inorganic Chemistry, 2013, 52, 11850-11858.	1.9	8
95	Spin valley and giant quantum spin Hall gap of hydrofluorinated bismuth nanosheet. Scientific Reports, 2018, 8, 7436.	1.6	8
96	Bulk electronic structure of Mn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub></mml:math>Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>/Ge(111) films by angle-resolved photoemission spectroscopy. Physical Review B, 2013, 87, .	1.1	6
97	Design of a polar half-metallic ferromagnet with accessible and enhanced electric polarization. Physical Review Materials, 2018, 2, .	0.9	6
98	Effect of Au proximity on the LSMO surface: An ab initio study. Journal of Magnetism and Magnetic Materials, 2012, 324, 2659-2663.	1.0	5
99	Simulation of Structural Phase Transitions in Perovskite Methylhydrazinium Metalâ€“Formate Frameworks: Coupled Ising and Potts Models. Journal of Physical Chemistry C, 2019, 123, 19912-19919.	1.5	5
100	Density functional theory study of single-molecule ferroelectricity in Preyssler-type polyoxometalates. APL Materials, 2021, 9, .	2.2	5
101	Chirality-induced spin texture switching in twisted bilayer graphene. Physical Review B, 2021, 104, .	1.1	5
102	Unravelling the Role of the Central Metal Ion in the Electronic Structure of Tris(8-hydroxyquinoline) Metal Chelates: Photoemission Spectroscopy and Hybrid Functional Calculations. Journal of Physical Chemistry A, 2012, 116, 11548-11552.	1.1	4
103	Modifying spin current filtering and magnetoresistance in a molecular spintronic device. RSC Advances, 2018, 8, 41587-41593.	1.7	4
104	Magnetic frustration in double perovskite LaSrNiRuO ₆. Europhysics Letters, 2018, 123, 57003.	0.7	4
105	First-principles study of the structural, electronic, magnetic, and ferroelectric properties of a charge-ordered iron(ii)-iron(iii) formate framework. Journal of Chemical Physics, 2019, 151, 124704.	1.2	4
106	Electronic structure of bimetallic Niâ€“Rh nanowires. Surface Science, 2010, 604, 1406-1413.	0.8	3
107	GiovannettietÂal.Reply:. Physical Review Letters, 2011, 107, .	2.9	3
108	Local probing of multiferroics: First-principles study of hyperfine parameters in YMnO₃and YMn₂O₅. EPJ Web of Conferences, 2014, 75, 09002.	0.1	3

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109	k dependence of the spin polarization inMn5Ge3/Ge(111)thin films. Physical Review B, 2015, 91, .	1.1	3
110	Analogies between Jahnâ€“Teller and Rashba spin physics. International Journal of Quantum Chemistry, 2016, 116, 1442-1450.	1.0	3
111	Molecular dynamics simulations of ferroelectricity in di-isopropyl-ammonium halide molecular crystals. Chemical Physics Letters, 2019, 730, 367-371.	1.2	3
112	Structural properties and stability of defected ZnSe/GaAs(001) interfaces. Computational Materials Science, 2005, 33, 256-262.	1.4	2
113	Possible High-T_C Layered Ferromagnetic Insulator Sr₂NiRuO₄: An Ab Initio Study. Journal of Physical Chemistry C, 2018, 122, 25589-25594.	1.5	2
114	Chirality and Magnetocaloricity in GdFeTeO6 as Compared to GdGaTeO6. Materials, 2021, 14, 5954.	1.3	2
115	Defect induced ferromagnetism in a two-dimensional metal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e357" altimg="si131.svg"><mml:mo>â^’</mml:mo></mml:math>organic framework. Journal of Magnetism and Magnetic Materials, 2022, 545, 168659.	1.0	2
116	First-Principles Study of Structure and Magnetism in Copper(II)-Containing Hybrid Perovskites. Crystals, 2020, 10, 1129.	1.0	1
117	2D hybrid CrCl2(N2C4H4)2 with tunable ferromagnetic half-metallicity. Journal of Materials Chemistry C, 2021, 9, 5985-5991.	2.7	1
118	Electronic Structure of Linear Polyacenes. Current Organic Chemistry, 2018, 21, .	0.9	1