Alessandro Stroppa

List of Publications by Citations

118 papers	5,846 citations	38 h-index	74 g-index
123 ext. papers	6,571 ext. citations	5 avg, IF	5.92 L-index

#	Paper	IF	Citations
118	Hybrid functionals applied to extended systems. *Journal of Physics Condensed Matter*, **2008**, 20, 064201	1.8	430
117	Accurate surface and adsorption energies from many-body perturbation theory. *Nature Materials*, **2010**, 9, 741-4	27	414
116	Hybrid improper ferroelectricity in a multiferroic and magnetoelectric metal-organic framework. *Advanced Materials*, **2013**, 25, 2284-90	24	246
115	Tuning the ferroelectric polarization in a multiferroic metal-organic framework. *Journal of the American Chemical Society*, **2013**, 135, 18126-30	16.4	225
114	Electric control of magnetization and interplay between orbital ordering and ferroelectricity in a multiferroic metal-organic framework. *Angewandte Chemie - International Edition*, **2011**, 50, 5847-50	16.4	223
113	Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites. *Nature Communications*, **2014**, 5, 5900	17.4	215
112	The shortcomings of semi-local and hybrid functionals: what we can learn from surface science studies. *New Journal of Physics*, **2008**, 10, 063020	2.9	209
111	Electronic structure and ferromagnetism of Mn-doped group-IV semiconductors. *Physical Review B*, **2003**, 68,	3.3	184
110	Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites. *Scientific Reports*, **2016**, 6, 28618	4.9	178
109	Ferroelectric Polarization of CH3NH3PbI3: A Detailed Study Based on Density Functional Theory and Symmetry Mode Analysis. *Journal of Physical Chemistry Letters*, **2015**, 6, 2223-31	6.4	151
108	Cross coupling between electric and magnetic orders in a multiferroic metal-organic framework. *Scientific Reports*, **2014**, 4, 6062	4.9	148
107	Hybrid functional study of proper and improper multiferroics. *Physical Chemistry Chemical Physics*, **2010**, 12, 5405-16	3.6	133
106	Spin-phonon coupling effects in transition-metal perovskites: A DFT + U and hybrid-functional study. *Physical Review B*, **2012**, 85,	3.3	126
105	Intrinsic and anisotropic Rashba spin splitting in Janus transition-metal dichalcogenide monolayers. *Physical Review B*, **2018**, 97,	3.3	124
104	CO adsorption on metal surfaces: A hybrid functional study with plane-wave basis set. *Physical Review B*, **2007**, 76,	3.3	121
103	Unraveling the Jahn-Teller effect in Mn-doped GaN using the Heyd-Scuseria-Ernzerhof hybrid functional. *Physical Review B*, **2009**, 79,	3.3	114
102	Emergence of ferroelectricity and spin-valley properties in two-dimensional honeycomb binary compounds. *Physical Review B*, **2015**, 91,	3.3	107

101	Magnetism in C- or N-doped MgO and ZnO: a density-functional study of impurity pairs. *Physical Review Letters*, **2010**, 105, 267203	7.4	103
100	The multiferroic phase of DyFeO3: anab initiostudy. *New Journal of Physics*, **2010**, 12, 093026	2.9	90
99	Experimental and theoretical studies of structural phase transition in a novel polar perovskite-like [C2H5NH3][Na0.5Fe0.5(HCOO)3] formate. *Dalton Transactions*, **2016**, 45, 2574-83	4.3	85
98	Multiferroicity in TTF-CA organic molecular crystals predicted through ab initio calculations. *Physical Review Letters*, **2009**, 103, 266401	7.4	85
97	Switchable electric polarization and ferroelectric domains in a metal-organic-framework. *Npj Quantum Materials*, **2016**, 1,	5	84
96	Large ferroelectric polarization in the new double perovskite NaLaMnWO6 induced by non-polar instabilities. *Physical Chemistry Chemical Physics*, **2011**, 13, 12186-90	3.6	83
95	Room-temperature polar order in [NH4][Cd(HCOO)3]--a hybrid inorganic-organic compound with a unique perovskite architecture. *Inorganic Chemistry*, **2015**, 54, 2109-16	5.1	69
94	High-T(c) ferroelectricity emerging from magnetic degeneracy in cupric oxide. *Physical Review Letters*, **2011**, 106, 026401	7.4	62
93	High-temperature ferroelectricity and strong magnetoelectric effects in a hybrid organic□inorganic perovskite framework. *Physica Status Solidi - Rapid Research Letters*, **2015**, 9, 62-67	2.5	59
92	Possibility of combining ferroelectricity and Rashba-like spin splitting in monolayers of the 1T-type transition-metal dichalcogenides MX2(M=Mo,W;X=S,Se,Te). *Physical Review B*, **2016**, 94,	3.3	59
91	Dielectric properties and magnetostriction of the collinear multiferroic spinel CdV2O4. *Physical Review B*, **2011**, 83,	3.3	59
90	Revisiting Mn-doped Ge using the Heyd-Scuseria-Ernzerhof hybrid functional. *Physical Review B*, **2011**, 83,	3.3	57
89	Strain tuning of ferroelectric polarization in hybrid organic inorganic perovskite compounds. *Journal of Physical Chemistry Letters*, **2015**, 6, 4553-9	6.4	55
88	Organic□inorganic hybrid perovskites ABI3 (A = CH3NH3, NH2CHNH2; B = Sn, Pb) as potential thermoelectric materials: a density functional evaluation. *RSC Advances*, **2015**, 5, 78701-78707	3.7	51
87	Electric Control of Magnetization and Interplay between Orbital Ordering and Ferroelectricity in a Multiferroic Metal□Organic Framework. *Angewandte Chemie*, **2011**, 123, 5969-5972	3.6	50
86	Zigzag antiferromagnetic quantum ground state in monoclinic honeycomb lattice antimonates A3Ni2SbO6(A=Li,Na). *Physical Review B*, **2015**, 92,	3.3	46
85	Coexistence of Three Ferroic Orders in the Multiferroic Compound [(CH3)4 N][Mn(N3)3] with Perovskite-Like Structure. *Chemistry - A European Journal*, **2016**, 22, 7863-70	4.8	46
84	Anharmonic lattice interactions in improper ferroelectrics for multiferroic design. *Journal of Physics Condensed Matter*, **2015**, 27, 283202	1.8	44

83	Polar distortions in hydrogen-bonded organic ferroelectrics. *Physical Review B*, **2011**, 84,	3.3	43
82	Polar Nature of (CHNH)BiI Perovskite-Like Hybrids. *Inorganic Chemistry*, **2017**, 56, 33-41	5.1	42
81	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. *Journal of Physical Chemistry C*, **2017**, 121, 23045-23054	3.8	39
80	Revealing the role of thiocyanate anion in layered hybrid halide perovskite (CHNH)Pb(SCN)I. *Journal of Chemical Physics*, **2017**, 146, 224702	3.9	38
79	Lone-Pair-Electron-Driven Ionic Displacements in a Ferroelectric Metal-Organic Hybrid. *Inorganic Chemistry*, **2016**, 55, 10337-10342	5.1	38
78	Anomalous and Polarization-Sensitive Photoresponse of T -WTe from Visible to Infrared Light. *Advanced Materials*, **2019**, 31, e1804629	24	37
77	Adsorption and Dissociation of CO on Bare and Ni-Decorated Stepped Rh(553) Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 942-949	3.8	36
76	Structural, electronic and ferroelectric properties of croconic acid crystal: a DFT study. *Physical Chemistry Chemical Physics*, **2012**, 14, 14673-81	3.6	35
75	Intertwined Rashba, Dirac, and Weyl Fermions in Hexagonal Hyperferroelectrics. *Physical Review Letters*, **2016**, 117, 076401	7.4	35
74	Exceptionally large room-temperature ferroelectric polarization in the PbNiO3 multiferroic nickelate: First-principles study. *Physical Review B*, **2012**, 86,	3.3	34
73	Advances in ab-initio theory of multiferroics. *European Physical Journal B*, **2012**, 85, 1	1.2	33
72	Magnetic phase transition and giant anisotropic magnetic entropy change in TbFeO3 single crystal. *Journal of Applied Physics*, **2016**, 119, 063904	2.5	32
71	Electric-Magneto-Optical Kerr Effect in a Hybrid Organic-Inorganic Perovskite. *Journal of the American Chemical Society*, **2017**, 139, 12883-12886	16.4	30
70	Ferroelectric polarization of hydroxyapatite from density functional theory. *RSC Advances*, **2017**, 7, 21375-21379	3.7	29
69	Composition and strain dependence of band offsets at metamorphic InxGa1−xAs/InyAl1−yAs heterostructures. *Physical Review B*, **2005**, 71,	3.3	29
68	Spin-reorientation magnetic transitions in Mn-doped SmFeO. *IUCrJ*, **2017**, 4, 598-603	4.7	29
67	Competing magnetic phases of Mn5Ge3 compound. *Physica Status Solidi (A) Applications and Materials Science*, **2007**, 204, 44-52	1.6	28
66	Computational and experimental imaging of Mn defects on GaAs (110) cross-sectional surfaces. *Physical Review B*, **2007**, 75,	3.3	28

65	Manipulation of valley pseudospin in WSe2/CrI3 heterostructures by the magnetic proximity effect. *Physical Review B*, **2020**, 101,	3.3	26
64	Tuning the ferroelectric polarization in AA′MnWO6 double perovskites through A cation substitution. *Dalton Transactions*, **2015**, 44, 10644-53	4.3	25
63	A RAIRS, TPD, and DFT Study of Carbon Monoxide Adsorption on Stepped Rh(553). *Journal of Physical Chemistry C*, **2008**, 112, 806-812	3.8	25
62	**2020**,		25
61	Magnetic Structures of Heterometallic M(II)-M(III) Formate Compounds. *Inorganic Chemistry*, **2017**, 56, 197-207	5.1	24
60	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	3.9	24
59	Brilliant triboluminescence in a potential organic–inorganic hybrid ferroelectric: (Ph3PO)2MnBr2. *Inorganic Chemistry Frontiers*, **2017**, 4, 154-159	6.8	22
58	Magneto-optical properties of (Ga,Mn)As: An ab initio determination. *Physical Review B*, **2008**, 77,	3.3	22
57	Ab initio study of the relation between electric polarization and electric field gradients in ferroelectrics. *Physical Review B*, **2012**, 86,	3.3	20
56	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	3.9	20
55	Improper ferroelectricity at antiferromagnetic domain walls of perovskite oxides. *Physical Review B* , **2017**, 96,	3.3	19
54	Lattice dynamics of Dirac node-line semimetal ZrSiS. *Physical Review B*, **2017**, 96,	3.3	19
53	Atomically precise semiconductor--graphene and hBN interfaces by Ge intercalation. *Scientific Reports*, **2015**, 5, 17700	4.9	19
52	Structural and ferroelectric transitions in magnetic nickelate PbNiO3. *New Journal of Physics*, **2014**, 16, 015030	2.9	19
51	Tuning the Weak Ferromagnetic States in Dysprosium Orthoferrite. *Scientific Reports*, **2016**, 6, 37529	4.9	19
50	Persistent Spin-texture and Ferroelectric Polarization in 2D Hybrid Perovskite Benzylammonium Lead-halide. *Journal of Physical Chemistry Letters*, **2020**, 11, 5177-5183	6.4	18
49	Bioferroelectric Properties of Glycine Crystals. *Journal of Physical Chemistry Letters*, **2019**, 10, 1319-1324	6.4	17
48	Electronic structure of tris(8-hydroxyquinolinato)aluminium(III) revisited using the Heyd-Scuseria-Ernzerhof hybrid functional: Theory and experiments. *Physical Review B*, **2011**, 84,	3.3	16

47	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. *Physical Review Materials*, **2019**, 3,	3.2	15
46	Ferroelectricity and ferromagnetism in a VOI2 monolayer: Role of the Dzyaloshinskii-Moriya interaction. *Physical Review B*, **2020**, 102,	3.3	15
45	Magneto-Optical Kerr Switching Properties of (CrI3)2 and (CrBr3/CrI3) Bilayers. *ACS Applied Electronic Materials*, **2020**, 2, 1373-1380	4	14
44	Spin polarization tuning in Mn5−xFexGe3. *Applied Physics Letters*, **2008**, 93, 092502	3.4	14
43	Tuning order-by-disorder multiferroicity in CuO by doping. *Physical Review B*, **2014**, 90,	3.3	13
42	On The Density Functional Theory Treatment of Lanthanide Coordination Compounds: A Comparative Study in a Series of Cu-Ln (Ln = Gd, Tb, Lu) Binuclear Complexes. *Inorganic Chemistry*, **2017**, 56, 9474-9485	5.1	13
41	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	13
40	Kinetic asymmetry in the growth of two-dimensional Mn oxide nanostripes. *Physical Review B*, **2013**, 88,	3.3	12
39	ZnSe□GaAs(001) heterostructures with defected interfaces: Structural, thermodynamic, and electronic properties. *Physical Review B*, **2005**, 72,	3.3	12
38	Switchable Rashba anisotropy in layered hybrid organic□inorganic perovskite by hybrid improper ferroelectricity. *Npj Computational Materials*, **2020**, 6,	10.9	12
37	Tunable spin textures in polar antiferromagnetic hybrid organic□inorganic perovskites by electric and magnetic fields. *Npj Computational Materials*, **2020**, 6,	10.9	12
36	Structural properties and strain engineering of a BeB2 monolayer from first-principles. *RSC Advances*, **2017**, 7, 38410-38414	3.7	11
35	Electronic transport of organic-inorganic hybrid perovskites from first-principles and machine learning. *Applied Physics Letters*, **2019**, 114, 083102	3.4	10
34	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	7.1	9
33	Structural and magnetic properties of Mn-doped GaAs(1 1 0) surface. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2006**, 126, 217-221	3.1	9
32	Magneto-electric coupling in antiferromagnet/ferroelectric Mn2Au/BaTiO3 interface. *Journal of Applied Physics*, **2016**, 120, 074104	2.5	9
31	Tuning the CO Dissociation Barriers by Low-Dimensional Surface Alloys. *Journal of Physical Chemistry C*, **2011**, 115, 21320-21323	3.8	8
30	Non-collinear magnetic states of Mn5Ge3 compound. *Materials Science in Semiconductor Processing*, **2006**, 9, 841-847	4.3	8

29	Two-dimensional metal dicyanamide frameworks of BeTriMe[M(dca)3(H2O)] (BeTriMe = benzyltrimethylammonium; dca = dicyanamide; M = Mn2+, Co2+, Ni2+): coexistence of polar and magnetic orders and nonlinear optical threshold temperature sensing. *Journal of Materials Chemistry C*, **2020**, 8, 11735-11747	7.1	8
28	Pressure-induced reversible framework rearrangement and increased polarization in the polar [NH4][Cd(HCOO)3] hybrid perovskite. *Inorganic Chemistry Frontiers*, **2019**, 6, 2379-2386	6.8	7
27	Synthesis and characterization of MnCrO4, a new mixed-valence antiferromagnet. *Inorganic Chemistry*, **2013**, 52, 11850-8	5.1	7
26	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	1.9	7
25	Bulk electronic structure of Mn5Ge3/Ge(111) films by angle-resolved photoemission spectroscopy. *Physical Review B*, **2013**, 87,	3.3	6
24	Cubic and tetragonal perovskites from the random phase approximation. *Physical Review Materials*, **2019**, 3,	3.2	6
23	Spin valley and giant quantum spin Hall gap of hydrofluorinated bismuth nanosheet. *Scientific Reports*, **2018**, 8, 7436	4.9	4
22	Effect of Au proximity on the LSMO surface: An ab initio study. *Journal of Magnetism and Magnetic Materials*, **2012**, 324, 2659-2663	2.8	4
21	Design of a polar half-metallic ferromagnet with accessible and enhanced electric polarization. *Physical Review Materials*, **2018**, 2,	3.2	4
20	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	3.9	3
19	Simulation of Structural Phase Transitions in Perovskite Methylhydrazinium Metal Formate Frameworks: Coupled Ising and Potts Models. *Journal of Physical Chemistry C*, **2019**, 123, 19912-19919	3.8	3
18	Local probing of multiferroics: First-principles study of hyperfine parameters in YMnO3and YMn2O5. *EPJ Web of Conferences*, **2014**, 75, 09002	0.3	3
17	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, 11548-52	2.8	3
16	Giovannetti et al. Reply:. *Physical Review Letters*, **2011**, 107,	7.4	3
15	Electronic structure of bimetallic NiRh nanowires. *Surface Science*, **2010**, 604, 1406-1413	1.8	3
14	k dependence of the spin polarization in Mn5Ge3/Ge(111) thin films. *Physical Review B*, **2015**, 91,	3.3	2
13	Analogies between Jahn Teller and Rashba spin physics. *International Journal of Quantum Chemistry*, **2016**, 116, 1442-1450	2.1	2
12	Modifying spin current filtering and magnetoresistance in a molecular spintronic device.. *RSC Advances*, **2018**, 8, 41587-41593	3.7	2

11	Magnetic frustration in double perovskite LaSrNiRuO 6. *Europhysics Letters*, **2018**, 123, 57003	1.6	2
10	Molecular dynamics simulations of ferroelectricity in di-isopropyl-ammonium halide molecular crystals. *Chemical Physics Letters*, **2019**, 730, 367-371	2.5	1
9	Structural properties and stability of defected ZnSe/GaAs(0 0 1) interfaces. *Computational Materials Science*, **2005**, 33, 256-262	3.2	1
8	Density functional theory study of single-molecule ferroelectricity in Preyssler-type polyoxometalates. *APL Materials*, **2021**, 9, 021109	5.7	1
7	Possible High-TC Layered Ferromagnetic Insulator Sr2NiRuO4: An Ab Initio Study. *Journal of Physical Chemistry C*, **2018**, 122, 25589-25594	3.8	1
6	Defect induced ferromagnetism in a two-dimensional metal□rganic framework. *Journal of Magnetism and Magnetic Materials*, **2021**, 545, 168659	2.8	0
5	2D hybrid CrCl2(N2C4H4)2 with tunable ferromagnetic half-metallicity. *Journal of Materials Chemistry C*, **2021**, 9, 5985-5991	7.1	0
4	First-Principles Study of Structure and Magnetism in Copper(II)-Containing Hybrid Perovskites. *Crystals*, **2020**, 10, 1129	2.3	
3	Hybrid Halide Perovskites **2020**, 15-78		
2	Hybrid Azide Perovskites **2020**, 151-179		
1	Hybrid Formate Perovskites **2020**, 79-149		