Alessio Filippetti

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

110 papers	5,284 citations	39 h-index	71 g-index
118 ext. papers	5,747 ext. citations	5.3 avg, IF	5.84 L-index

#	Paper	IF	Citations
110	Theoretical insight on PTB7:PC71BM, PTB7-th:PC71BM and Si-PCPDTBT:PC71BM interactions governing blend nanoscale morphology for efficient solar cells. *Nano Energy*, **2021**, 82, 105708	17.1	3
109	Fundamentals of tin iodide perovskites: a promising route to highly efficient, lead-free solar cells. *Journal of Materials Chemistry A*, **2021**, 9, 11812-11826	13	12
108	Long-lived electrets and lack of ferroelectricity in methylammonium lead bromide CHNHPbBr ferroelastic single crystals. *Physical Chemistry Chemical Physics*, **2021**, 23, 3233-3245	3.6	4
107	Ag/In lead-free double perovskites. *EcoMat*, **2020**, 2, e12017	9.4	12
106	Artificial quantum confinement in LaAlO3/SrTiO3 heterostructures. *Physical Review Materials*, **2020**, 4,	3.2	4
105	The dominant role of surfaces in the hysteretic behavior of hybrid perovskites. *Nano Energy*, **2020**, 67, 104162	17.1	12
104	A three-order-parameter bistable magnetoelectric multiferroic metal. *Nature Communications*, **2020**, 11, 4922	17.4	4
103	Influence of thermal conductivity and of non-constant relaxation time on thermoelectricity in Mg3Sb2. *Journal of Physics: Conference Series*, **2019**, 1226, 012010	0.3	2
102	Layered Germanium Hybrid Perovskite Bromides: Insights from Experiments and First-Principles Calculations. *Advanced Functional Materials*, **2019**, 29, 1903528	15.6	17
101	How far does the defect tolerance of lead-halide perovskites range? The example of Bi impurities introducing efficient recombination centers. *Journal of Materials Chemistry A*, **2019**, 7, 23838-23853	13	38
100	Singling out the effect of quenched disorder in the phase diagram of cuprates. *Journal of Physics Condensed Matter*, **2019**, 31, 184002	1.8	1
99	Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH3NH3PbI3 Perovskites. *Journal of Physical Chemistry C*, **2019**, 123, 6753-6762	3.8	2
98	Theory of thermoelectricity in MgSb with an energy- and temperature-dependent relaxation time. *Journal of Physics Condensed Matter*, **2019**, 31, 065702	1.8	8
97	Meta-screening and permanence of polar distortion in metallized ferroelectrics. *Physical Review B*, **2018**, 97,	3.3	24
96	Study of equilibrium carrier transfer in LaAlO3/SrTiO3 from an epitaxial La1− Sr x MnO3 ferromagnetic layer. *Journal of Physics Communications*, **2018**, 2, 025010	1.2	2
95	Strain-induced magnetization control in an oxide multiferroic heterostructure. *Physical Review B*, **2018**, 97,	3.3	17
94	Ab-Initio Calculations of TMO Band Structure. *Springer Series in Materials Science*, **2018**, 181-213	0.9	

93	Electronic properties of fluorides by efficient approximated quasiparticle DFT-1/2 and PSIC methods: BaF, CaF and CdF as test cases. *Journal of Physics Condensed Matter*, **2018**, 30, 365501	1.8	13
92	Charge doping and large lattice expansion in oxygen-deficient heteroepitaxial WO3. *Physical Review Materials*, **2018**, 2,	3.2	14
91	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. *Advanced Materials Interfaces*, **2018**, 6, 1801173	4.6	13
90	Conductivity and Local Structure of LaNiO Thin Films. *Advanced Materials*, **2017**, 29, 1605197	24	36
89	Collective Molecular Mechanisms in the CHNHPbI Dissolution by Liquid Water. *ACS Nano*, **2017**, 11, 9183-9190	13.7	49
88	Photoluminescence, optical gain, and lasing threshold in CH3NH3PbI3 methylammonium lead-halide perovskites obtained by ab initio calculations. *Journal of Materials Chemistry C*, **2017**, 5, 12758-12768	7.1	4
87	Insulator-to-Metal Transition at Oxide Interfaces Induced by WO Overlayers. *ACS Applied Materials & Interfaces*, **2017**, 9, 42336-42343	9.5	5
86	Modeling hybrid perovskites by molecular dynamics. *Journal of Physics Condensed Matter*, **2017**, 29, 043001	2.8	45
85	Structure and Thermodynamic Properties of Hybrid Perovskites by Classical Molecular Dynamics **2017**, 1-42		
84	Large phonon-drag enhancement induced by narrow quantum confinement at the LaAlO3/SrTiO3 interface. *Physical Review B*, **2016**, 93,	3.3	8
83	Polaronic metal state at the LaAlO3/SrTiO3 interface. *Nature Communications*, **2016**, 7, 10386	17.4	99
82	Prediction of a native ferroelectric metal. *Nature Communications*, **2016**, 7, 11211	17.4	48
81	Thermally Activated Point Defect Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultrahigh Mobility of Iodine. *Journal of Physical Chemistry Letters*, **2016**, 7, 2356-61	6.4	93
80	Temperature Evolution of Methylammonium Trihalide Vibrations at the Atomic Scale. *Journal of Physical Chemistry Letters*, **2016**, 7, 529-35	6.4	66
79	Theoretical and experimental investigation of optical absorption anisotropy in □Ga2O3. *Journal of Physics Condensed Matter*, **2016**, 28, 224005	1.8	46
78	Appealing Perspectives of Hybrid Lead□bdide Perovskites as Thermoelectric Materials. *Journal of Physical Chemistry C*, **2016**, 120, 28472-28479	3.8	49
77	Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide CH3NH3PbI3 perovskites. *Physical Chemistry Chemical Physics*, **2016**, 18, 15352-62	3.6	68
76	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. *Physical Chemistry Chemical Physics*, **2016**, 18, 24318-24	3.6	41

75	Methylammonium Rotational Dynamics in Lead Halide Perovskite by Classical Molecular Dynamics: The Role of Temperature. *Journal of Physical Chemistry C*, **2015**, 119, 17421-17428	3.8	200
74	Intrinsic origin of two-dimensional electron gas at the (001) surface of SrTiO3. *Physical Review B*, **2015**, 91,	3.3	24
73	Entropy-Suppressed Ferroelectricity in Hybrid Lead-Iodide Perovskites. *Journal of Physical Chemistry Letters*, **2015**, 6, 4909-15	6.4	47
72	Methylammonium fragmentation in amines as source of localized trap levels and the healing role of Cl in hybrid lead-iodide perovskites. *Physical Review B*, **2015**, 92,	3.3	53
71	Giant oscillating thermopower at oxide interfaces. *Nature Communications*, **2015**, 6, 6678	17.4	52
70	Doping-dependent band structure of LaAlO3/SrTiO3 interfaces by soft x-ray polarization-controlled resonant angle-resolved photoemission. *Physical Review B*, **2014**, 89,	3.3	61
69	Radiative Recombination and Photoconversion of Methylammonium Lead Iodide Perovskite by First Principles: Properties of an Inorganic Semiconductor within a Hybrid Body. *Journal of Physical Chemistry C*, **2014**, 118, 24843-24853	3.8	69
68	Structural and ferroelectric transitions in magnetic nickelate PbNiO3. *New Journal of Physics*, **2014**, 16, 015030	2.9	19
67	Multigap absorption in CaCu3Ti4O12 and the prediction capability of ab initio methods. *Physical Review B*, **2014**, 90,	3.3	2
66	Hybrid perovskites for photovoltaics: Insights from first principles. *Physical Review B*, **2014**, 89,	3.3	168
65	Multiferroicity in vanadium-doped La2Ti2O7: insights from first principles. *European Physical Journal B*, **2013**, 86, 1	1.2	10
64	Surface antiferromagnetism and incipient metal-insulator transition in strained manganite films. *Physical Review B*, **2013**, 87,	3.3	8
63	Giant electroresistance and tunable magnetoelectricity in a multiferroic junction. *Physical Review B*, **2013**, 88,	3.3	3
62	Large band offset as driving force of two-dimensional electron confinement: The case of SrTiO3/SrZrO3 interface. *Physical Review B*, **2013**, 88,	3.3	22
61	Doping-induced dimensional crossover and thermopower burst in Nb-doped SrTiO3 superlattices. *Physical Review B*, **2013**, 88,	3.3	34
60	Ferromagnetism and orbital order in a topological ferroelectric. *Physical Review Letters*, **2012**, 109, 217202	7.4	19
59	Thermopower in oxide heterostructures: The importance of being multiple-band conductors. *Physical Review B*, **2012**, 86,	3.3	43
58	Exceptionally large room-temperature ferroelectric polarization in the PbNiO3 multiferroic nickelate: First-principles study. *Physical Review B*, **2012**, 86,	3.3	34

57	Ordering and multiple phase transitions in ultrathin nickelate superlattices. *Physical Review B*, **2012**, 86,	3.3	34
56	Exceptionally strong magnetism in the 4d perovskites RTcO3 (R=Ca, Sr, Ba). *Physical Review B*, **2011**, 83,	3.3	39
55	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods. *Physical Review B*, **2011**, 84,	3.3	53
54	Spontaneous 2-dimensional carrier confinement at the n-type SrTiO3/LaAlO3 interface. *Physical Review Letters*, **2011**, 106, 166807	7.4	170
53	Variational pseudo-self-interaction-corrected density functional approach to the ab initio description of correlated solids and molecules. *Physical Review B*, **2011**, 84,	3.3	71
52	First-principles calculation of electronic and structural properties of YBa2Cu3O6+y. *Physical Review B*, **2010**, 82,	3.3	15
51	Multiferroicity and orbital ordering in Pr0.5Ca0.5MnO3 from first principles. *Physical Review B*, **2010**, 82,	3.3	13
50	Band alignment at Cu2O/La0.7Sr0.3MnO3 interface: A combined experimental-theoretical determination. *Applied Physics Letters*, **2010**, 97, 032115	3.4	11
49	Dielectric and vibrational properties of bixbyite sesquioxides. *Physical Review B*, **2009**, 80,	3.3	6
48	Fermi-surface pockets in YBa2Cu3O6.5: Comparison of ab initio techniques. *Physical Review B*, **2009**, 79,	3.3	9
47	Fermi-surface pockets in magnetic underdoped cuprates from first principles. *Europhysics Letters*, **2009**, 88, 67009	1.6	2
46	Magnetic couplings vs. stress and strain in epitaxial (La, Sr)MnO3. *European Physical Journal B*, **2009**, 70, 343-346	1.2	4
45	A practical first-principles band-theory approach to the study of correlated materials. *European Physical Journal B*, **2009**, 71, 139-183	1.2	40
44	Jahn-Teller stabilization of magnetic and orbital ordering in rocksalt CuO. *Physical Review B*, **2009**, 80,	3.3	21
43	Chain metallicity and competition between paramagnetism and antiferromagnetism in underdoped YBa2Cu3O6+x: A first principles description. *Physical Review B*, **2008**, 78,	3.3	12
42	Interplay of strain and magnetism in La1−xSrxMnO3 from first principles. *Physical Review B*, **2008**, 78,	3.3	33
41	Metal-insulator transitions and singlet polarons in one-dimensional Ca2+xY2−xCu5O10. *Physical Review B*, **2008**, 77,	3.3	9
40	Dielectric constant boost in amorphous sesquioxides. *Applied Physics Letters*, **2008**, 92, 172903	3.4	14

39	Conservation of dielectric constant upon amorphization in perovskite oxides. *Physical Review B*, **2007**, 76,	3.3	10
38	Self-interaction-free density-functional band theory for magnetic cuprates. *Journal of Magnetism and Magnetic Materials*, **2007**, 310, 1648-1650	2.8	5
37	Cation charge anomalies and high-□dielectric behavior in DyScO3: Ab initio density-functional and self-interaction-corrected calculations. *Physical Review B*, **2007**, 75,	3.3	31
36	Magnetism of La0.625Sr0.375MnO3 under high pressure from first principles. *Physical Review B*, **2007**, 76,	3.3	29
35	Magnetic ordering under strain and spin-Peierls dimerization in GeCuO3. *Physical Review Letters*, **2007**, 98, 196403	7.4	15
34	A Theoretical View on the Dielectric Properties of Crystalline and Amorphous High-□Materials and Films **2007**, 269-292		1
33	Electronic Structure of Bulk and Defected CaCu3Ti4O12. *ECS Transactions*, **2006**, 3, 291-297	1	5
32	Double-exchange driven ferromagnetic metal-paramagnetic insulator transition in Mn-doped CuO. *Physical Review B*, **2006**, 74,	3.3	24
31	Dielectric properties and long-wavelength optical modes of the high-□oxide LaAlO3. *Physical Review B*, **2005**, 71,	3.3	61
30	Coexistence of ionic and metallic bonding in noble-metal oxides. *Physical Review B*, **2005**, 72,	3.3	61
29	Self-interaction errors in density-functional calculations of electronic transport. *Physical Review Letters*, **2005**, 95, 146402	7.4	277
28	Magnetic ordering in CuO from first principles: a cuprate antiferromagnet with fully three-dimensional exchange interactions. *Physical Review Letters*, **2005**, 95, 086405	7.4	82
27	Strong correlation and ferromagnetism in (Ga,Mn)As and (Ga,Mn)N. *Journal of Magnetism and Magnetic Materials*, **2005**, 290-291, 1391-1394	2.8	11
26	Self-interaction effects in (Ga,Mn)As and (Ga,Mn)N. *Chemical Physics*, **2005**, 309, 59-65	2.3	36
25	Pseudopotential Method **2005**, 431-440		
24	The origin of ferroelectricity in magnetoelectric YMnO3. *Nature Materials*, **2004**, 3, 164-70	27	948
23	Self-interaction-corrected pseudopotential scheme for magnetic and strongly-correlated systems. *Physical Review B*, **2003**, 67,	3.3	230
22	Strong-correlation effects in Born effective charges. *Physical Review B*, **2003**, 68,	3.3	53

21	Why are there any magnetic ferroelectrics?. *Journal of Magnetism and Magnetic Materials*, **2002**, 242-245, 976-979	2.8	209
20	Coexistence of magnetism and ferroelectricity in perovskites. *Physical Review B*, **2002**, 65,	3.3	163
19	First principles study of structural, electronic and magnetic interplay in ferroelectromagnetic yttrium manganite. *Journal of Magnetism and Magnetic Materials*, **2001**, 236, 176-189	2.8	54
18	Stress and reconstruction on (001) transition-metal surfaces. *Computational Materials Science*, **2001** , 20, 423-428	3.2	3
17	Double-exchange-driven spin pairing at the (001) surface of manganites. *Physical Review B*, **2000**, 62, 11571-11575	3.3	32
16	Theory and applications of the stress density. *Physical Review B*, **2000**, 61, 8433-8442	3.3	109
15	Magnetic stress as a driving force of structural distortions: the case of CrN. *Physical Review Letters*, **2000**, 85, 5166-9	7.4	101
14	Electron doping in the honeycomb bilayer superconductors (Zr, Hf)NCl. *Europhysics Letters*, **1999**, 48, 320-325	1.6	86
13	Magnetic Reconstruction at the (001) CaMnO3 Surface. *Physical Review Letters*, **1999**, 83, 4184-4187	7.4	22
12	Competition between magnetic and structural transitions in CrN. *Physical Review B*, **1999**, 59, 7043-7050	3.3	82
11	Prediction of a ferromagnetic ground state for NaCl-type FeN. *Physical Review B*, **1999**, 59, 8397-8400	3.3	27
10	Anomalous relaxations and chemical trends at III-V semiconductor nitride nonpolar surfaces. *Physical Review B*, **1999**, 59, 8026-8031	3.3	56
9	Faceting and stress of missing-row reconstructed transition-metal (110) surfaces. *Physical Review B*, **1999**, 60, 14366-14371	3.3	15
8	Ionicity and Relaxation Anomalies at III□V Nitride Surfaces. *Physica Status Solidi A*, **1998**, 170, 265-269		8
7	Electron affinity in density-functional theory in the local-spin-density approximation. *Physical Review A*, **1998**, 57, 914-919	2.6	16
6	Reconstructions of Ir(110) and (100): an ab initio study. *Surface Science*, **1997**, 377-379, 112-116	1.8	45
5	Hardness conservation as a new transferability criterion: Application to fully nonlocal pseudopotentials. *International Journal of Quantum Chemistry*, **1997**, 61, 421-427	2.1	7
4	Chemical hardness, linear response, and pseudopotential transferability. *Physical Review B*, **1995**, 52, 11793-11804	3.3	58

3	Formation Energy, Stress, and Relaxations of Low-Index Rhodium Surfaces. *Materials Research Society Symposia Proceedings*, **1995**, 408, 457	3
2	Dielectric Properties of Rare-Earth Oxides: General Trends from Theory225-246	2
1	Nanosession: 2D Electron Systems - Electronic Structure and Field Effects89-97	