

Alessio Filippetti

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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	The origin of ferroelectricity in magnetoelectric YMnO ₃ . <i>Nature Materials</i> , 2004 , 3, 164-70	27	948
109	Self-interaction errors in density-functional calculations of electronic transport. <i>Physical Review Letters</i> , 2005 , 95, 146402	7.4	277
108	Self-interaction-corrected pseudopotential scheme for magnetic and strongly-correlated systems. <i>Physical Review B</i> , 2003 , 67,	3.3	230
107	Why are there any magnetic ferroelectrics?. <i>Journal of Magnetism and Magnetic Materials</i> , 2002 , 242-245, 976-979	2.8	209
106	Methylammonium Rotational Dynamics in Lead Halide Perovskite by Classical Molecular Dynamics: The Role of Temperature. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 17421-17428	3.8	200
105	Spontaneous 2-dimensional carrier confinement at the n-type SrTiO ₃ /LaAlO ₃ interface. <i>Physical Review Letters</i> , 2011 , 106, 166807	7.4	170
104	Hybrid perovskites for photovoltaics: Insights from first principles. <i>Physical Review B</i> , 2014 , 89,	3.3	168
103	Coexistence of magnetism and ferroelectricity in perovskites. <i>Physical Review B</i> , 2002 , 65,	3.3	163
102	Theory and applications of the stress density. <i>Physical Review B</i> , 2000 , 61, 8433-8442	3.3	109
101	Magnetic stress as a driving force of structural distortions: the case of CrN. <i>Physical Review Letters</i> , 2000 , 85, 5166-9	7.4	101
100	Polaronic metal state at the LaAlO ₃ /SrTiO ₃ interface. <i>Nature Communications</i> , 2016 , 7, 10386	17.4	99
99	Thermally Activated Point Defect Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultrahigh Mobility of Iodine. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2356-61	6.4	93
98	Electron doping in the honeycomb bilayer superconductors (Zr, Hf)NCl. <i>Europhysics Letters</i> , 1999 , 48, 320-325	1.6	86
97	Magnetic ordering in CuO from first principles: a cuprate antiferromagnet with fully three-dimensional exchange interactions. <i>Physical Review Letters</i> , 2005 , 95, 086405	7.4	82
96	Competition between magnetic and structural transitions in CrN. <i>Physical Review B</i> , 1999 , 59, 7043-7050	3.3	82
95	Variational pseudo-self-interaction-corrected density functional approach to the ab initio description of correlated solids and molecules. <i>Physical Review B</i> , 2011 , 84,	3.3	71
94	Radiative Recombination and Photoconversion of Methylammonium Lead Iodide Perovskite by First Principles: Properties of an Inorganic Semiconductor within a Hybrid Body. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 24843-24853	3.8	69

93	Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide CH ₃ NH ₃ PbI ₃ perovskites. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 15352-62	3.6	68
92	Temperature Evolution of Methylammonium Trihalide Vibrations at the Atomic Scale. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 529-35	6.4	66
91	Doping-dependent band structure of LaAlO ₃ /SrTiO ₃ interfaces by soft x-ray polarization-controlled resonant angle-resolved photoemission. <i>Physical Review B</i> , 2014 , 89,	3.3	61
90	Dielectric properties and long-wavelength optical modes of the high- κ oxide LaAlO ₃ . <i>Physical Review B</i> , 2005 , 71,	3.3	61
89	Coexistence of ionic and metallic bonding in noble-metal oxides. <i>Physical Review B</i> , 2005 , 72,	3.3	61
88	Chemical hardness, linear response, and pseudopotential transferability. <i>Physical Review B</i> , 1995 , 52, 11793-11804	3.3	58
87	Anomalous relaxations and chemical trends at III-V semiconductor nitride nonpolar surfaces. <i>Physical Review B</i> , 1999 , 59, 8026-8031	3.3	56
86	First principles study of structural, electronic and magnetic interplay in ferroelectromagnetic yttrium manganite. <i>Journal of Magnetism and Magnetic Materials</i> , 2001 , 236, 176-189	2.8	54
85	Methylammonium fragmentation in amines as source of localized trap levels and the healing role of Cl in hybrid lead-iodide perovskites. <i>Physical Review B</i> , 2015 , 92,	3.3	53
84	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods. <i>Physical Review B</i> , 2011 , 84,	3.3	53
83	Strong-correlation effects in Born effective charges. <i>Physical Review B</i> , 2003 , 68,	3.3	53
82	Giant oscillating thermopower at oxide interfaces. <i>Nature Communications</i> , 2015 , 6, 6678	17.4	52
81	Collective Molecular Mechanisms in the CH ₃ NH ₃ PbI ₃ Dissolution by Liquid Water. <i>ACS Nano</i> , 2017 , 11, 9183-9190	16.7	49
80	Appealing Perspectives of Hybrid Lead-Iodide Perovskites as Thermoelectric Materials. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 28472-28479	3.8	49
79	Prediction of a native ferroelectric metal. <i>Nature Communications</i> , 2016 , 7, 11211	17.4	48
78	Entropy-Suppressed Ferroelectricity in Hybrid Lead-Iodide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4909-15	6.4	47
77	Theoretical and experimental investigation of optical absorption anisotropy in BiGa ₂ O ₃ . <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 224005	1.8	46
76	Modeling hybrid perovskites by molecular dynamics. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 043003	3.0	45

75	Reconstructions of Ir(110) and (100): an ab initio study. <i>Surface Science</i> , 1997 , 377-379, 112-116	1.8	45
74	Thermopower in oxide heterostructures: The importance of being multiple-band conductors. <i>Physical Review B</i> , 2012 , 86,	3.3	43
73	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 24318-24	3.6	41
72	A practical first-principles band-theory approach to the study of correlated materials. <i>European Physical Journal B</i> , 2009 , 71, 139-183	1.2	40
71	Exceptionally strong magnetism in the 4d perovskites RTcO ₃ (R=Ca, Sr, Ba). <i>Physical Review B</i> , 2011 , 83,	3.3	39
70	How far does the defect tolerance of lead-halide perovskites range? The example of Bi impurities introducing efficient recombination centers. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 23838-23853	1.3	38
69	Conductivity and Local Structure of LaNiO Thin Films. <i>Advanced Materials</i> , 2017 , 29, 1605197	2.4	36
68	Self-interaction effects in (Ga,Mn)As and (Ga,Mn)N. <i>Chemical Physics</i> , 2005 , 309, 59-65	2.3	36
67	Exceptionally large room-temperature ferroelectric polarization in the PbNiO ₃ multiferroic nickelate: First-principles study. <i>Physical Review B</i> , 2012 , 86,	3.3	34
66	Doping-induced dimensional crossover and thermopower burst in Nb-doped SrTiO ₃ superlattices. <i>Physical Review B</i> , 2013 , 88,	3.3	34
65	Ordering and multiple phase transitions in ultrathin nickelate superlattices. <i>Physical Review B</i> , 2012 , 86,	3.3	34
64	Interplay of strain and magnetism in La _{1-x} Sr _x MnO ₃ from first principles. <i>Physical Review B</i> , 2008 , 78,	3.3	33
63	Double-exchange-driven spin pairing at the (001) surface of manganites. <i>Physical Review B</i> , 2000 , 62, 11571-11575	3.3	32
62	Cation charge anomalies and high- ϵ dielectric behavior in DyScO ₃ : Ab initio density-functional and self-interaction-corrected calculations. <i>Physical Review B</i> , 2007 , 75,	3.3	31
61	Magnetism of La _{0.625} Sr _{0.375} MnO ₃ under high pressure from first principles. <i>Physical Review B</i> , 2007 , 76,	3.3	29
60	Prediction of a ferromagnetic ground state for NaCl-type FeN. <i>Physical Review B</i> , 1999 , 59, 8397-8400	3.3	27
59	Intrinsic origin of two-dimensional electron gas at the (001) surface of SrTiO ₃ . <i>Physical Review B</i> , 2015 , 91,	3.3	24
58	Meta-screening and permanence of polar distortion in metallized ferroelectrics. <i>Physical Review B</i> , 2018 , 97,	3.3	24

57	Double-exchange driven ferromagnetic metal-paramagnetic insulator transition in Mn-doped CuO. <i>Physical Review B</i> , 2006 , 74,	3.3	24
56	Large band offset as driving force of two-dimensional electron confinement: The case of SrTiO ₃ /SrZrO ₃ interface. <i>Physical Review B</i> , 2013 , 88,	3.3	22
55	Magnetic Reconstruction at the (001) CaMnO ₃ Surface. <i>Physical Review Letters</i> , 1999 , 83, 4184-4187	7.4	22
54	Jahn-Teller stabilization of magnetic and orbital ordering in rocksalt CuO. <i>Physical Review B</i> , 2009 , 80,	3.3	21
53	Structural and ferroelectric transitions in magnetic nickelate PbNiO ₃ . <i>New Journal of Physics</i> , 2014 , 16, 015030	2.9	19
52	Ferromagnetism and orbital order in a topological ferroelectric. <i>Physical Review Letters</i> , 2012 , 109, 217204	2.4	19
51	Layered Germanium Hybrid Perovskite Bromides: Insights from Experiments and First-Principles Calculations. <i>Advanced Functional Materials</i> , 2019 , 29, 1903528	15.6	17
50	Strain-induced magnetization control in an oxide multiferroic heterostructure. <i>Physical Review B</i> , 2018 , 97,	3.3	17
49	Electron affinity in density-functional theory in the local-spin-density approximation. <i>Physical Review A</i> , 1998 , 57, 914-919	2.6	16
48	First-principles calculation of electronic and structural properties of YBa ₂ Cu ₃ O _{6+y} . <i>Physical Review B</i> , 2010 , 82,	3.3	15
47	Magnetic ordering under strain and spin-Peierls dimerization in GeCuO ₃ . <i>Physical Review Letters</i> , 2007 , 98, 196403	7.4	15
46	Faceting and stress of missing-row reconstructed transition-metal (110) surfaces. <i>Physical Review B</i> , 1999 , 60, 14366-14371	3.3	15
45	Dielectric constant boost in amorphous sesquioxides. <i>Applied Physics Letters</i> , 2008 , 92, 172903	3.4	14
44	Charge doping and large lattice expansion in oxygen-deficient heteroepitaxial WO ₃ . <i>Physical Review Materials</i> , 2018 , 2,	3.2	14
43	Electronic properties of fluorides by efficient approximated quasiparticle DFT-1/2 and PSIC methods: BaF, CaF and CdF as test cases. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 365501	1.8	13
42	Multiferroicity and orbital ordering in Pr _{0.5} Ca _{0.5} MnO ₃ from first principles. <i>Physical Review B</i> , 2010 , 82,	3.3	13
41	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. <i>Advanced Materials Interfaces</i> , 2018 , 6, 1801173	4.6	13
40	Ag/In lead-free double perovskites. <i>EcoMat</i> , 2020 , 2, e12017	9.4	12

39	Chain metallicity and competition between paramagnetism and antiferromagnetism in underdoped YBa ₂ Cu ₃ O _{6+x} : A first principles description. <i>Physical Review B</i> , 2008 , 78,	3.3	12
38	The dominant role of surfaces in the hysteretic behavior of hybrid perovskites. <i>Nano Energy</i> , 2020 , 67, 104162	17.1	12
37	Fundamentals of tin iodide perovskites: a promising route to highly efficient, lead-free solar cells. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 11812-11826	13	12
36	Band alignment at Cu ₂ O/La _{0.7} Sr _{0.3} MnO ₃ interface: A combined experimental-theoretical determination. <i>Applied Physics Letters</i> , 2010 , 97, 032115	3.4	11
35	Strong correlation and ferromagnetism in (Ga,Mn)As and (Ga,Mn)N. <i>Journal of Magnetism and Magnetic Materials</i> , 2005 , 290-291, 1391-1394	2.8	11
34	Multiferroicity in vanadium-doped La ₂ Ti ₂ O ₇ : insights from first principles. <i>European Physical Journal B</i> , 2013 , 86, 1	1.2	10
33	Conservation of dielectric constant upon amorphization in perovskite oxides. <i>Physical Review B</i> , 2007 , 76,	3.3	10
32	Fermi-surface pockets in YBa ₂ Cu ₃ O _{6.5} : Comparison of ab initio techniques. <i>Physical Review B</i> , 2009 , 79,	3.3	9
31	Metal-insulator transitions and singlet polarons in one-dimensional Ca _{2+x} Y ₂ Cu ₅ O ₁₀ . <i>Physical Review B</i> , 2008 , 77,	3.3	9
30	Large phonon-drag enhancement induced by narrow quantum confinement at the LaAlO ₃ /SrTiO ₃ interface. <i>Physical Review B</i> , 2016 , 93,	3.3	8
29	Surface antiferromagnetism and incipient metal-insulator transition in strained manganite films. <i>Physical Review B</i> , 2013 , 87,	3.3	8
28	Ionicity and Relaxation Anomalies at III-V Nitride Surfaces. <i>Physica Status Solidi A</i> , 1998 , 170, 265-269		8
27	Theory of thermoelectricity in MgSb with an energy- and temperature-dependent relaxation time. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 065702	1.8	8
26	Hardness conservation as a new transferability criterion: Application to fully nonlocal pseudopotentials. <i>International Journal of Quantum Chemistry</i> , 1997 , 61, 421-427	2.1	7
25	Dielectric and vibrational properties of bixbyite sesquioxides. <i>Physical Review B</i> , 2009 , 80,	3.3	6
24	Insulator-to-Metal Transition at Oxide Interfaces Induced by WO ₃ Overlayers. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 42336-42343	9.5	5
23	Self-interaction-free density-functional band theory for magnetic cuprates. <i>Journal of Magnetism and Magnetic Materials</i> , 2007 , 310, 1648-1650	2.8	5
22	Electronic Structure of Bulk and Defected CaCu ₃ Ti ₄ O ₁₂ . <i>ECS Transactions</i> , 2006 , 3, 291-297	1	5

21	Photoluminescence, optical gain, and lasing threshold in CH ₃ NH ₃ PbI ₃ methylammonium lead-halide perovskites obtained by ab initio calculations. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 12758-12768	7.1	4
20	Magnetic couplings vs. stress and strain in epitaxial (La, Sr)MnO ₃ . <i>European Physical Journal B</i> , 2009 , 70, 343-346	1.2	4
19	Artificial quantum confinement in LaAlO ₃ /SrTiO ₃ heterostructures. <i>Physical Review Materials</i> , 2020 , 4,	3.2	4
18	A three-order-parameter bistable magnetoelectric multiferroic metal. <i>Nature Communications</i> , 2020 , 11, 4922	17.4	4
17	Long-lived electrets and lack of ferroelectricity in methylammonium lead bromide CH ₃ NH ₃ PbBr ferroelastic single crystals. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 3233-3245	3.6	4
16	Giant electroresistance and tunable magnetoelectricity in a multiferroic junction. <i>Physical Review B</i> , 2013 , 88,	3.3	3
15	Stress and reconstruction on (001) transition-metal surfaces. <i>Computational Materials Science</i> , 2001 , 20, 423-428	3.2	3
14	Formation Energy, Stress, and Relaxations of Low-Index Rhodium Surfaces. <i>Materials Research Society Symposia Proceedings</i> , 1995 , 408, 457		3
13	Theoretical insight on PTB7:PC71BM, PTB7-th:PC71BM and Si-PCPDTBT:PC71BM interactions governing blend nanoscale morphology for efficient solar cells. <i>Nano Energy</i> , 2021 , 82, 105708	17.1	3
12	Influence of thermal conductivity and of non-constant relaxation time on thermoelectricity in Mg ₃ Sb ₂ . <i>Journal of Physics: Conference Series</i> , 2019 , 1226, 012010	0.3	2
11	Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH ₃ NH ₃ PbI ₃ Perovskites. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 6753-6762	3.8	2
10	Study of equilibrium carrier transfer in LaAlO ₃ /SrTiO ₃ from an epitaxial La _{1-x} Sr _x MnO ₃ ferromagnetic layer. <i>Journal of Physics Communications</i> , 2018 , 2, 025010	1.2	2
9	Multigap absorption in CaCu ₃ Ti ₄ O ₁₂ and the prediction capability of ab initio methods. <i>Physical Review B</i> , 2014 , 90,	3.3	2
8	Fermi-surface pockets in magnetic underdoped cuprates from first principles. <i>Europhysics Letters</i> , 2009 , 88, 67009	1.6	2
7	Dielectric Properties of Rare-Earth Oxides: General Trends from Theory	225-246	2
6	Singling out the effect of quenched disorder in the phase diagram of cuprates. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 184002	1.8	1
5	A Theoretical View on the Dielectric Properties of Crystalline and Amorphous High-κ Materials and Films	2007 , 269-292	1
4	Ab-Initio Calculations of TMO Band Structure. <i>Springer Series in Materials Science</i> , 2018 , 181-213	0.9	

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