Alessio Filippetti

List of Publications by Year
in descending order

116 papers	6,193 citations	70961 41 h-index	69108 77 g-index
118 all docs	118 docs citations	118 times ranked	7557 citing authors

#	Article	IF	Citations
1	The origin of ferroelectricity in magnetoelectric YMnO3. Nature Materials, 2004, 3, 164-170.	13.3	1,081
2	Self-Interaction Errors in Density-Functional Calculations of Electronic Transport. Physical Review Letters, 2005, 95, 146402.	2.9	292
3	Methylammonium Rotational Dynamics in Lead Halide Perovskite by Classical Molecular Dynamics: The Role of Temperature. Journal of Physical Chemistry C, 2015, 119, 17421-17428.	1.5	255
4	Self-interaction-corrected pseudopotential scheme for magnetic and strongly-correlated systems. Physical Review B, 2003, 67, .	1.1	242
5	Why are there any magnetic ferroelectrics?. Journal of Magnetism and Magnetic Materials, 2002, 242-245, 976-979.	1.0	228
6	Hybrid perovskites for photovoltaics: Insights from first principles. Physical Review B, 2014, 89, .	1.1	191
7	Spontaneous 2-Dimensional Carrier Confinement at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-Type<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Interface. Physical Review Letters, 2011, 106, 166807.	2.9	185
8	Coexistence of magnetism and ferroelectricity in perovskites. Physical Review B, 2002, 65, .	1.1	173
9	Theory and applications of the stress density. Physical Review B, 2000, 61, 8433-8442.	1.1	139
10	Polaronic metal state at the LaAlO3/SrTiO3 interface. Nature Communications, 2016, 7, 10386.	5.8	130
11	Thermally Activated Point Defect Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultrahigh Mobility of Iodine. Journal of Physical Chemistry Letters, 2016, 7, 2356-2361.	2.1	125
12	Magnetic Stress as a Driving Force of Structural Distortions: The Case of CrN. Physical Review Letters, 2000, 85, 5166-5169.	2.9	114
13	Electron doping in the honeycomb bilayer superconductors (Zr, Hf)NCl. Europhysics Letters, 1999, 48, 320-325.	0.7	91
14	Competition between magnetic and structural transitions in CrN. Physical Review B, 1999, 59, 7043-7050.	1.1	91
15	Magnetic Ordering in CuO from First Principles: A Cuprate Antiferromagnet with Fully Three-Dimensional Exchange Interactions. Physical Review Letters, 2005, 95, 086405.	2.9	89
16	Chemical hardness, linear response, and pseudopotential transferability. Physical Review B, 1995, 52, 11793-11804.	1.1	83
17	Variational pseudo-self-interaction-corrected density functional approach to theab initiodescription of correlated solids and molecules. Physical Review B, 2011, 84, .	1.1	83
18	Temperature Evolution of Methylammonium Trihalide Vibrations at the Atomic Scale. Journal of Physical Chemistry Letters, 2016, 7, 529-535.	2.1	82

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19	Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide CH₃NH₃PbI₃perovskites. Physical Chemistry Chemical Physics, 2016, 18, 15352-15362.	1.3	77
20	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.	1.5	74
21	Collective Molecular Mechanisms in the CH₃NH₃PbI₃ Dissolution by Liquid Water. ACS Nano, 2017, 11, 9183-9190.	7.3	73
22	Prediction of a native ferroelectric metal. Nature Communications, 2016, 7, 11211.	5.8	71
23	Doping dependent band structure of LaAlO <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>/SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>interfaces by soft x-ray polarization-controlled resonant angle-resolved photoemission. Physical Review B, 2014, 89, .	1.1	70
24	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advancedab initiomethods. Physical Review B, 2011, 84, .	1.1	66
25	Appealing Perspectives of Hybrid Leadâ€“Iodide Perovskites as Thermoelectric Materials. Journal of Physical Chemistry C, 2016, 120, 28472-28479.	1.5	66
26	Modeling hybrid perovskites by molecular dynamics. Journal of Physics Condensed Matter, 2017, 29, 043001.	0.7	66
27	Dielectric properties and long-wavelength optical modes of the high-îºoxideLaAlO3. Physical Review B, 2005, 71, .	1.1	65
28	Coexistence of ionic and metallic bonding in noble-metal oxides. Physical Review B, 2005, 72, .	1.1	64
29	Conductivity and Local Structure of LaNiO₃ Thin Films. Advanced Materials, 2017, 29, 1605197.	11.1	63
30	Anomalous relaxations and chemical trends at III-V semiconductor nitride nonpolar surfaces. Physical Review B, 1999, 59, 8026-8031.	1.1	62
31	Giant oscillating thermopower at oxide interfaces. Nature Communications, 2015, 6, 6678.	5.8	62
32	Theoretical and experimental investigation of optical absorption anisotropy in Î²-Ga₂O₃. Journal of Physics Condensed Matter, 2016, 28, 224005.	0.7	59
33	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.	5.2	57
34	First principles study of structural, electronic and magnetic interplay in ferroelectromagnetic yttrium manganite. Journal of Magnetism and Magnetic Materials, 2001, 236, 176-189.	1.0	56
35	Strong-correlation effects in Born effective charges. Physical Review B, 2003, 68, .	1.1	56
36	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, .	1.1	54

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37	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. Physical Chemistry Chemical Physics, 2016, 18, 24318-24324.	1.3	52
38	Entropy-Suppressed Ferroelectricity in Hybrid Lead-Iodide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 4909-4915.	2.1	51
39	Thermopower in oxide heterostructures: The importance of being multiple-band conductors. Physical Review B, 2012, 86, .	1.1	48
40	Reconstructions of Ir(110) and (100): an ab initio study. Surface Science, 1997, 377-379, 112-116.	0.8	47
41	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. Advanced Materials Interfaces, 2019, 6, 1801173.	1.9	43
42	A practical first-principles band-theory approach to the study of correlated materials. European Physical Journal B, 2009, 71, 139-183.	0.6	42
43	Electronic and magnetic properties of 4<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>d</mml:mi></mml:mrow></mml:math>perovskites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>R</mml:mi></mml:mrow></mml:math>TcO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow /><mml:msub><mml:mi	1.1	42
44	Ordering and multiple phase transitions in ultrathin nickelate superlattices. Physical Review B, 2012, 86, .	1.1	41
45	Doping-induced dimensional crossover and thermopower burst in Nb-doped SrTiO<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>superlattices. Physical Review B, 2013, 88, .	1.1	40
46	Meta-screening and permanence of polar distortion in metallized ferroelectrics. Physical Review B, 2018, 97, .	1.1	39
47	Self-interaction effects in (Ga,Mn)As and (Ga,Mn)N. Chemical Physics, 2005, 309, 59-65.	0.9	38
48	Interplay of strain and magnetism inLa1âˆ'xSrxMnO3from first principles. Physical Review B, 2008, 78, .	1.1	36
49	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
50	Cation charge anomalies and high-Îºdielectric behavior inDyScO3:Ab initiodensity-functional and self-interaction-corrected calculations. Physical Review B, 2007, 75, .	1.1	34
51	Double-exchange-driven spin pairing at the (001) surface of manganites. Physical Review B, 2000, 62, 11571-11575.	1.1	32
52	Fundamentals of tin iodide perovskites: a promising route to highly efficient, lead-free solar cells. Journal of Materials Chemistry A, 2021, 9, 11812-11826.	5.2	32
53	Magnetism of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">La</mml:mi><mml:mn>0.625</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Sr</mml:mi><mml:mn>0.375</mml:mn></mml:msub><mml:mi mathvariant="normal">Mn</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>under	1.1	31
54	Prediction of a ferromagnetic ground state for NaCl-type FeN. Physical Review B, 1999, 59, 8397-8400.	1.1	27

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55	Intrinsic origin of two-dimensional electron gas at the (001) surface of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>SrTiO</mml:mtext><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2015, 91, .	1.1	27
56	Magnetic Reconstruction at the (001)CaMnO3Surface. Physical Review Letters, 1999, 83, 4184-4187.	2.9	26
57	Double-exchange driven ferromagnetic metal-paramagnetic insulator transition in Mn-doped CuO. Physical Review B, 2006, 74, .	1.1	26
58	Strain-induced magnetization control in an oxide multiferroic heterostructure. Physical Review B, 2018, 97, .	1.1	26
59	Layered Germanium Hybrid Perovskite Bromides: Insights from Experiments and Firstâ€Principles Calculations. Advanced Functional Materials, 2019, 29, 1903528.	7.8	26
60	Jahn-Teller stabilization of magnetic and orbital ordering in rocksalt CuO. Physical Review B, 2009, 80, .	1.1	25
61	Large band offset as driving force of two-dimensional electron confinement: The case of SrTiO<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>/SrZrO<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>interface. Physical Review B, 2013, 88, .	1.1	25
62	The dominant role of surfaces in the hysteretic behavior of hybrid perovskites. Nano Energy, 2020, 67, 104162.	8.2	24
63	Structural and ferroelectric transitions in magnetic nickelate PbNiO₃. New Journal of Physics, 2014, 16, 015030.	1.2	23
64	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	1.9	23
65	Ferromagnetism and Orbital Order in a Topological Ferroelectric. Physical Review Letters, 2012, 109, 217202.	2.9	21
66	Electron affinity in density-functional theory in the local-spin-density approximation. Physical Review A, 1998, 57, 914-919.	1.0	18
67	Charge doping and large lattice expansion in oxygen-deficient heteroepitaxial <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">WO</mml:mi><mml:mn mathvariant="bold">3</mml:mn></mml:msub></mml:math>. Physical Review Materials, 2018, 2, .	0.9	18
68	First-principles calculation of electronic and structural properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YBa</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2010, 82, .	1.1	17
69	Magnetic Ordering under Strain and Spin-Peierls Dimerization inGeCuO3. Physical Review Letters, 2007, 98, 196403.	2.9	16
70	Dielectric constant boost in amorphous sesquioxides. Applied Physics Letters, 2008, 92, .	1.5	16
71	Electronic properties of fluorides by efficient approximated quasiparticle DFT-1/2 and PSIC methods: BaF₂, CaF₂and CdF₂as test cases. Journal of Physics Condensed Matter, 2018, 30, 365501.	0.7	16
72	Ag/In leadâ€free double perovskites. EcoMat, 2020, 2, e12017.	6.8	16

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73	Faceting and stress of missing-row reconstructed transition-metal (110) surfaces. Physical Review B, 1999, 60, 14366-14371.	1.1	15
74	Theory of thermoelectricity in Mg₃Sb₂ with an energy- and temperature-dependent relaxation time. Journal of Physics Condensed Matter, 2019, 31, 065702.	0.7	15
75	Multiferroicity and orbital ordering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Pr</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn> first principles. Physical Review B, 2010, 82, .	1.1	14
76	Chain metallicity and competition between paramagnetism and antiferromagnetism in underdoped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YBa</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms A first principles de. Physical Review B, 2008, 78, .	1.1	13
77	Strong correlation and ferromagnetism in (Ga,Mn)As and (Ga,Mn)N. Journal of Magnetism and Magnetic Materials, 2005, 290-291, 1391-1394.	1.0	12
78	Multiferroicity in vanadium-doped La2Ti2O7: insights from first principles. European Physical Journal B, 2013, 86, 1.	0.6	12
79	Fermi-surface pockets in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YBa</mml:mtext></mml:mrow><mml:mn>2</mml:mn> Comparison ofab initiotechniques. Physical Review B, 2009, 79, .	1.1	11
80	Band alignment at Cu2O/La0.7Sr0.3MnO3 interface: A combined experimental-theoretical determination. Applied Physics Letters, 2010, 97, .	1.5	11
81	Surface antiferromagnetism and incipient metal-insulator transition in strained manganite films. Physical Review B, 2013, 87, .	1.1	11
82	Conservation of dielectric constant upon amorphization in perovskite oxides. Physical Review B, 2007, 76, .	1.1	10
83	Metal-insulator transitions and singlet polarons in one-dimensional<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ca</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review B, 2008, 77, .	1.1	9
84	Large phonon-drag enhancement induced by narrow quantum confinement at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></m Physical Review B, 2016, 93, .	1.1	9
85	Ionicity and Relaxation Anomalies at IIIâ€“V Nitride Surfaces. Physica Status Solidi A, 1998, 170, 265-269.	1.7	8
86	Dielectric and vibrational properties of bixbyite sesquioxides. Physical Review B, 2009, 80, .	1.1	8
87	A three-order-parameter bistable magnetoelectric multiferroic metal. Nature Communications, 2020, 11, 4922.	5.8	8
88	Hardness conservation as a new transferability criterion: Application to fully nonlocal pseudopotentials. International Journal of Quantum Chemistry, 1997, 61, 421-427.	1.0	7
89	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.	8.2	7
90	Long-lived electrets and lack of ferroelectricity in methylammonium lead bromide CH₃NH₃PbBr₃ ferroelastic single crystals. Physical Chemistry Chemical Physics, 2021, 23, 3233-3245.	1.3	7

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91	Direct measurement of radiative decay rates in metal halide perovskites. Energy and Environmental Science, 2022, 15, 1211-1221.	15.6	7
92	Insulator-to-Metal Transition at Oxide Interfaces Induced by WO₃ Overlayers. ACS Applied Materials & Interfaces, 2017, 9, 42336-42343.	4.0	6
93	Artificial quantum confinement in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LaAl</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> heterostructures. Physical Review Materials, 2020, 4, .	3.1	6
94	Electronic Structure of Bulk and Defected CaCu3Ti4O12. ECS Transactions, 2006, 3, 291-297.	0.3	5
95	Self-interaction-free density-functional band theory for magnetic cuprates. Journal of Magnetism and Magnetic Materials, 2007, 310, 1648-1650.	1.0	5
96	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.	2.7	5
97	Formation Energy, Stress, and Relaxations of Low-Index Rhodium Surfaces. Materials Research Society Symposia Proceedings, 1995, 408, 457.	0.1	4
98	Magnetic couplings vs. stress and strain in epitaxial (La, Sr)MnO3. European Physical Journal B, 2009, 70, 343-346.	0.6	4
99	Study of equilibrium carrier transfer in LaAlO₃/SrTiO₃ from an epitaxial La_{1â^'x}Sr_xMnO₃ ferromagnetic layer. Journal of Physics Communications, 2018, 2, 025010.	0.5	4
100	Stress and reconstruction on (001) transition-metal surfaces. Computational Materials Science, 2001, 20, 423-428.	1.4	3
101	Giant electroresistance and tunable magnetoelectricity in a multiferroic junction. Physical Review B, 2013, 88, .	1.1	3
102	Influence of thermal conductivity and of non-constant relaxation time on thermoelectricity in Mg₃Sb₂. Journal of Physics: Conference Series, 2019, 1226, 012010.	0.3	3
103	Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH₃NH₃PbI₃ Perovskites. Journal of Physical Chemistry C, 2019, 123, 6753-6762.	1.5	3
104	Dielectric Properties of Rare-Earth Oxides: General Trends from Theory. , 0, , 225-246.		2
105	Fermi-surface pockets in magnetic underdoped cuprates from first principles. Europhysics Letters, 2009, 88, 67009.	0.7	2
106	Multigap absorption inCaCu3Ti4O12and the prediction capability ofab initiomethods. Physical Review B, 2014, 90, .	1.1	2
107	Electronic Structure Of Defects In Dielectrics With Electronic Correlation. ECS Transactions, 2006, 3, 267-275.	0.3	1
108	Singling out the effect of quenched disorder in the phase diagram of cuprates. Journal of Physics Condensed Matter, 2019, 31, 184002.	0.7	1

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109	A Theoretical View on the Dielectric Properties of Crystalline and Amorphous High-Îº Materials and Films. , 2007, , 269-292.		1
110	Pseudopotential Method. , 2005, , 431-440.		0
111	Exchange-interactions and chemical bonding in CuO by first-principles. , 2005, , .		0
112	Dielectric Properties of High-K Materials : a Theoretical View. ECS Transactions, 2006, 3, 309-314.	0.3	0
113	Electronic properties and doping mechanism in cuprates by first-principles calculations. , 2008, , .		0
114	Publisher's Note: Dielectric and vibrational properties of bixbyite sesquioxides [Phys. Rev. B80, 104301 (2009)]. Physical Review B, 2009, 80, .	1.1	0
115	Ab-Initio Calculations of TMO Band Structure. Springer Series in Materials Science, 2018, , 181-213.	0.4	0
116	Structure and Thermodynamic Properties of Hybrid Perovskites by Classical Molecular Dynamics. , 2017, , 1-42.		0