

Cesare Franchini

List of Publications by Year in descending order

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150
papers

8,914
citations

61857

43
h-index

43802

91
g-index

154
all docs

154
docs citations

154
times ranked

11280
citing authors

#	ARTICLE	IF	CITATIONS
19	Behavior of Methylammonium Dipoles in MAPbX ₃ (X = Br and I). Journal of Physical Chemistry Letters, 2017, 8, 4113-4121.	2.1	103
20	Charge Trapping at the Step Edges of TiO ₂ Anatase (101). Angewandte Chemie - International Edition, 2014, 53, 4714-4716.	7.2	102
21	Anisotropic two-dimensional electron gas at SrTiO ₃ (110). Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3933-3937.	3.3	99
22	Polaronic Hole Trapping in Doped BaBiO ₃ . Physical Review Letters, 2009, 102, 256402.	2.9	93
23	Local Structure and Coordination Define Adsorption in a Model Ir ₁ Fe ₃ O ₄ Single-Atom Catalyst. Angewandte Chemie - International Edition, 2019, 58, 13961-13968.	7.2	93
24	Polarity compensation mechanisms on the perovskite surface KTaO ₃ (001). Science, 2018, 359, 572-575.	6.0	85
25	Coexistence of trapped and free excess electrons in SrTiO ₃ . Physical Review B, 2015, 91, .	3.3	83
26	Hybrid functionals applied to perovskites. Journal of Physics Condensed Matter, 2014, 26, 253202.	0.7	81
27	Structural, vibrational, and quasiparticle properties of the Peierls semiconductor BaBiO ₃ : A hybrid functional and self-consistent GW+vertex-corrections study. Physical Review B, 2010, 81, .	1.1	79
28	Water agglomerates on Fe ₃ O ₄ (001). Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E5642-E5650.	3.3	79
29	Interplay between Adsorbates and Polarons: CO on Rutile TiO ₂ . Physical Review B, 2015, 92, .	2.1	77
30	Anisotropic magnetic couplings and structure-driven canted to collinear transitions in Sr ₂ MnO ₇ : magnetically constrained noncollinear DFT. Physical Review B, 2015, 92, .	2.1	77
31	Electronic, optical, and mechanical properties of superhard cold-compressed phases of carbon. Applied Physics Letters, 2011, 99, .	1.5	68
32	Formation and dynamics of small polarons on the rutile TiO ₂ (110) surface. Physical Review B, 2018, 98, .	1.1	67
33	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods. Physical Review B, 2011, 84, .	1.1	66
34	Electronic structure of PbFe _{1/2} Ta _{1/2} O ₃ : Crystallographic ordering and magnetic properties. Physical Review B, 2004, 69, .	1.1	64
35	Formation of Mn ₃ O ₄ on SrTiO ₃ surface: Surface and interface structural stability. Physical Review B, 2007, 76, .	1.1	62
36	Room-temperature dynamic correlation between methylammonium molecules in lead-iodine based perovskites: An <i>ab initio</i> molecular dynamics perspective. Physical Review B, 2016, 94, .	1.1	62

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37	Density functional study of the polar MnO(111) surface. Physical Review B, 2006, 73, .	1.1	61
38	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. Journal of Physical Chemistry C, 2017, 121, 23045-23054.	1.5	56
39	Three-Dimensional Electronic Structure of the Type-II Weyl Semimetal WTe_2 Physical Review Letters, 2017, 119, 026403.	2.9	55
40	Influence of surface atomic structure demonstrated on oxygen incorporation mechanism at a model perovskite oxide. Nature Communications, 2018, 9, 3710.	5.8	54
41	Donor defects and small polarons on the TiO ₂ (110) surface. Journal of Applied Physics, 2016, 119, .	1.1	51
42	Epitaxial stabilization of MnO(111) overlayers on a Pd(100) surface. Physical Review B, 2007, 75, .	1.1	47
43	Superconducting properties of MgB ₂ from first principles. Physica C: Superconductivity and Its Applications, 2007, 456, 45-53.	0.6	46
44	The random phase approximation applied to ice. Journal of Chemical Physics, 2014, 140, 084502.	1.2	45
45	Converged quasiparticle energies for transition metal oxide perovskites. Physical Review Materials, 2018, 2, .	0.9	45
46	Local Structure and Coordination Define Adsorption in a Model Ir ₁ Fe ₃ O ₄ Single-Atom Catalyst. Angewandte Chemie, 2019, 131, 14099-14106.	1.6	44
47	Structure of the c(2 $\sqrt{2}$ -2)-Br/Pt(110) surface. Physical Review B, 2002, 65, .	1.1	43
48	Structural and vibrational properties of two-dimensional Mn _x on Pd(100): Experiments and density functional theory calculations. Physical Review B, 2009, 79, .	1.1	42
49	Structural and vibrational properties of two-dimensional perovskites R _d TcO ₃ Physical Review B, 2009, 79, .	1.1	42
50	Ab initio prediction of pressure-induced superconductivity in potassium. Physical Review B, 2006, 73, .	1.1	41
51	Ab initio study of the structural, electronic, and magnetic properties of MnO(100) and MnO(110). Physical Review B, 2007, 75, .	1.1	41
52	Relativistic +BSE study of the optical properties of Ruddlesden-Popper iridates. Physical Review Materials, 2018, 2, .	0.9	40
53	Resolving the adsorption of molecular O ₂ on the rutile TiO ₂ (110) surface by noncontact atomic force microscopy. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 14827-14837.	3.3	39
54	Tuning the vertical location of helical surface states in topological insulator heterostructures via dual-proximity effects. Scientific Reports, 2013, 3, 1233.	1.6	38

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55	Dimensionality-strain phase diagram of strontium iridates. <i>Physical Review B</i> , 2017, 95, .	1.1	37
56	Structural transitions and transport-half-metallic ferromagnetism in LaMnO_3 at elevated pressure. <i>Physical Review B</i> , 2012, 85, .	1.1	36
57	Exceptionally large room-temperature ferroelectric polarization in the PbNiO_3 multiferroic nickelate: First-principles study. <i>Physical Review B</i> , 2012, 86, .	1.1	36
58	Two-dimensional manganese oxide nanolayers on Pd(100): the surface phase diagram. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 134008.	0.7	35
59	Proton Ordering of Cubic Ice Ic: Spectroscopy and Computer Simulations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 10989-10997.	1.5	35
60	Parametrization of $\text{LSDA} + \text{U}$ for noncollinear magnetic configurations: Multipolar magnetism in UO_2 . <i>Physical Review Materials</i> , 2019, 3, .	0.9	35
61	Lifshitz transition driven by spin fluctuations and spin-orbit renormalization in NaOsO_3 . <i>Physical Review B</i> , 2016, 94, .	1.1	34
62	Large enhancement of the photovoltaic effect in ferroelectric complex oxides through bandgap reduction. <i>Scientific Reports</i> , 2016, 6, 28313.	1.6	34
63	Assessing the performance of self-consistent hybrid functional for band gap calculation in oxide semiconductors. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 454004.	0.7	33
64	Interplay between magnetic, electronic, and vibrational effects in monolayer Mn_3O_4 grown on Pd(100). <i>Journal of Chemical Physics</i> , 2009, 130, 124707.	1.2	32
65	Strain-driven onset of nontrivial topological insulating states in ZrIn_2Sb compounds		

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73	Strained $c(4\text{\AA}-2)$ CoO(100)-like monolayer on Pd(100): Experiment and theory. Surface Science, 2010, 604, 529-534.	0.8	27
74	Electron and hole doping in the relativistic Mott insulator Sr^2IrO_4 : A first-principles study using Lithium Niobate-Type Oxides as Visible Light Photovoltaic Materials. Chemistry of Materials, 2016, 28, 25-29.	1.1	27
75	Diagrammatic Monte Carlo study of Fröhlich polaron dispersion in two and three dimensions. Physical Review B, 2018, 97, .	3.2	26
76	Diagrammatic Monte Carlo study of Fröhlich polaron dispersion in two and three dimensions. Physical Review B, 2018, 97, .	1.1	26
77	Halogen-Induced Corrosion of Platinum. Journal of the American Chemical Society, 2009, 131, 2827-2829.	6.6	25
78	Anisotropy of magnetic interactions and symmetry of the order parameter in unconventional superconductor Sr_2RuO_4 . Npj Quantum Materials, 2017, 2, .	1.8	24
79	$(3\text{\AA}-1)\text{-Br/Pt}(110)$ structure and the charge-density-wave-assisted $c(2\text{\AA}-2)$ to $(3\text{\AA}-1)$ phase transition. Physical Review B, 2004, 69, .	1.1	23
80	Structural and ferroelectric transitions in magnetic nickelate PbNiO_3 . New Journal of Physics, 2014, 16, 015030.	1.2	23
81	Combined first-principles and model Hamiltonian study of the perovskite series R_3MnO_7		

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91	Structural, Electronic, and Ferroelectric Properties of Compressed CdPbO ₃ Polymorphs. Inorganic Chemistry, 2013, 52, 1032-1039.	1.9	14
92	Vacancy clusters at domain boundaries and band bending at the SrTiO_3 surface. Physical Review B, 2014, 90, .	1.1	14
93	Stabilizing Single Ni Adatoms on a Two-Dimensional Porous Titania Overlayer at the SrTiO ₃ (110) Surface. Journal of Physical Chemistry C, 2014, 118, 19904-19909.	1.5	14
94	Structural determination and electronic properties of the 4dperovskite SrPdO ₃ . Physical Review B, 2014, 89, .	1.1	14
95	Interplay between multipolar spin interactions, Jahn-Teller effect, and electronic correlation in a $\text{J}^{\text{eff}}=1$ insulator. Physical Review B, 2021, 103, .	1.1	14
96	Electronic State Unfolding for Plane Waves: Energy Bands, Fermi Surfaces, and Spectral Functions. Journal of Physical Chemistry C, 2021, 125, 12921-12928.	1.5	14
97	CO oxidation by Pt ₂ /Fe ₃ O ₄ : Metastable dimer and support configurations facilitate lattice oxygen extraction. Science Advances, 2022, 8, eabn4580.	4.7	14
98	Intriguing electronic and optical properties of M ₂ CX ₂ (M ⁻ =Mo, W; X ⁻ =O, F) MXenes and their van der Waals heterostructures. Chemical Physics Letters, 2019, 731, 136614.	1.2	13
99	Superconductivity in SrTiO ₃ : Dielectric Function Method for Non-Parabolic Bands. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2739-2744.	0.8	12
100	Chemical Pressure-Induced Ferromagnetism and Stabilization of the Metallic State in Ba _{1-x} Sr _x VS ₃ . International Journal of Modern Physics B, 2003, 17, 3503-3508.	1.0	11
101	Phase transitions driven by competing interactions in low-dimensional systems. Europhysics Letters, 2010, 92, 26004.	0.7	11
102	Ru doping in iron-based pnictides: The unfolded dominant role of structural effects for superconductivity. Physical Review B, 2017, 95, .	1.1	11
103	Influence of Local Defects on the Dynamics of H Bond Breaking and Formation on a Magnetite Surface. Journal of Physical Chemistry C, 2019, 123, 19742-19747.	1.5	11
104	CuAu, a hexagonal two-dimensional metal. 2D Materials, 2020, 7, 045017.	2.0	11
105	Kagome metal-organic frameworks as a platform for strongly correlated electrons. JPhys Materials, 2020, 3, 025001.	1.8	11
106	Comparative <i>ab initio</i> study of the structural, electronic, magnetic, and dynamical properties of LiOsO_3 and NaOsO_3 .	0.9	11
107	and NaOsO_3 and LiOsO_3 .	2.9	10
108	Electron-phonon interactions using the projector augmented-wave method and Wannier functions. Physical Review B, 2020, 101, .	1.1	10

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109	Small Polarons in Transition Metal Oxides. , 2020, , 1035-1073.		10
110	Cubic and tetragonal perovskites from the random phase approximation. Physical Review Materials, 2019, 3, .	0.9	10
111	Doping Evolution of the Local Electronic and Structural Properties of the Double Perovskite $\text{Ba}_{2-x}\text{Na}_x\text{Ca}_x\text{OsO}_6$. Journal of Physical Chemistry C, 2020, 124, 16577-16585.	1.5	9
112	Optical and excitonic properties of transition metal oxide perovskites by the Bethe-Salpeter equation. Physical Review Materials, 2021, 5, .	0.9	9
113	Structural, transport, and electronic properties of a layered dichalcogenide AuVS_2 with semimetallic properties. Physical Review B, 2002, 66, .	1.1	8
114	Role of electronic correlations on the ground-state properties and on the pressure-induced metal-insulator transition in BaVS_3 . Physical Review B, 2004, 70, .	1.1	8
115	Thickness dependent structural and electronic properties of CuO grown on $\text{SrTiO}_3(100)$: a hybrid density functional theory study. Journal of Physics Condensed Matter, 2011, 23, 045004.	0.7	8
116	Covalent effects in magnetic ferroelectrics $\text{MnM}_3\text{O}_{12}$ ($\text{M} = \text{Ti, Sn}$). Physica Status Solidi (B): Basic Research, 2015, 252, 626-634.	0.7	8
117	Competing magnetic interactions in a spin- $\frac{1}{2}$ square lattice: Hidden order in Sr_2VO_4 . Physical Review B, 2017, 96, .	1.1	8
118	Ab initio prediction of the high-pressure phase diagram of BaBiO_3 . Physical Review B, 2017, 96, .	1.1	8
119	Rapid oxygen exchange between hematite and water vapor. Nature Communications, 2021, 12, 6488.	5.8	8
120	Machine learning for exploring small polaron configurational space. Npj Computational Materials, 2022, 8, .	3.5	8
121	First-principles investigation of $\text{BaFe}_2\text{As}_2(001)$. Physical Review B, 2010, 82, .	1.1	7
122	Tailor-made ultrathin manganese oxide nanostripes: \sim magic widths \sim on $\text{Pd}(1\ 1\text{N})$ terraces. Journal of Physics Condensed Matter, 2012, 24, 042001.	0.7	7
123	Experimental observation of defect pair separation triggering phase transitions. Scientific Reports, 2014, 4, 4110.	1.6	7
124	Optical Response of an Interacting Polaron Gas in Strongly Polar Crystals. Applied Sciences (Switzerland), 2020, 10, 2059.	1.3	7
125	Modeling magnetic multipolar phases in density functional theory. Physical Review B, 2022, 106, .	1.1	7
126	Electronically driven phase transitions in a quasi-one-dimensional adsorbate system. European Physical Journal B, 2010, 75, 15-22.	0.6	6

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145	Challenges and Opportunities in Modeling Oxides for Energy and Information Devices. , 2020, , 1001-1012.		2
146	Revealing the quasiparticle electronic and excitonic nature in cubic, tetragonal, and hexagonal phases of FAPbI_3 . AIP Advances, 2022, 12, 025330.	0.6	2
147	Low Dimensionality and Epitaxial Stabilization in Metal-Supported Oxide Nanostructures: Mnx Oy on Pd(100) Mnx Oy . Springer Series in Materials Science, 2012, , 209-237.	0.4	0
148	Challenges and Opportunities in Modeling Oxides for Energy and Information Devices. , 2019, , 1-13.		0
149	Special issue on novel superconducting and magnetic materials. Journal of Physics Condensed Matter, 2020, 32, 040401.	0.7	0
150	Defect chemistry of Eu dopants in NaI scintillators studied by atomically resolved force microscopy. Physical Review Materials, 2019, 3, .	0.9	0