Cesare Franchini

List of Publications by Citations

142 papers	6,742 citations	40 h-index	79 g-index
154 ext. papers	7,906 ext. citations	5.4 avg, IF	6.08 L-index

#	Paper	IF	Citations
142	Dirac semimetal and topological phase transitions in A3Bi (A=Na, K, Rb). *Physical Review B*, **2012**, 85,	3.3	1244
141	Stacking effects on the electronic and optical properties of bilayer transition metal dichalcogenides MoS2, MoSe2, WS2, and WSe2. *Physical Review B*, **2014**, 89,	3.3	328
140	Role of self-trapping in luminescence and p-type conductivity of wide-band-gap oxides. *Physical Review B*, **2012**, 85,	3.3	328
139	Direct view at excess electrons in TiO2 rutile and anatase. *Physical Review Letters*, **2014**, 113, 086402	7.4	300
138	Ground-state properties of multivalent manganese oxides: Density functional and hybrid density functional calculations. *Physical Review B*, **2007**, 75,	3.3	259
137	Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites. *Nature Communications*, **2014**, 5, 5900	17.4	215
136	Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites. *Scientific Reports*, **2016**, 6, 28618	4.9	178
135	Density functional theory study of MnO by a hybrid functional approach. *Physical Review B*, **2005**, 72,	3.3	147
134	Superconductivity in lithium, potassium, and aluminum under extreme pressure: a first-principles study. *Physical Review Letters*, **2006**, 96, 047003	7.4	138
133	Dual behavior of excess electrons in rutile TiO2. *Physica Status Solidi - Rapid Research Letters*, **2013**, 7, 199-203	2.5	126
132	Screened hybrid functional applied to 3d0-â3d8 transition-metal perovskites LaMO3 (M = Sc□u): Influence of the exchange mixing parameter on the structural, electronic, and magnetic properties. *Physical Review B*, **2012**, 86,	3.3	124
131	Superconducting properties of MgB2 from first principles. *Physical Review Letters*, **2005**, 94, 037004	7.4	122
130	Hardness of T-carbon: Density functional theory calculations. *Physical Review B*, **2011**, 84,	3.3	120
129	Charge trapping at the step edges of TiO(2) anatase (101). *Angewandte Chemie - International Edition*, **2014**, 53, 4714-6	16.4	90
128	Maximally localized Wannier functions in LaMnO3 within PBE + U, hybrid functionals and partially self-consistent GW: an efficient route to construct ab initio tight-binding parameters for eg perovskites. *Journal of Physics Condensed Matter*, **2012**, 24, 235602	1.8	88
127	Anisotropic two-dimensional electron gas at SrTiO3(110). *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 3933-7	11.5	83
126	Rocksalt SnS and SnSe: Native topological crystalline insulators. *Physical Review B*, **2013**, 88,	3.3	79

125	Polaronic hole trapping in doped BaBiO3. *Physical Review Letters*, **2009**, 102, 256402	7.4	77
124	Behavior of Methylammonium Dipoles in MAPbX (X = Br and I). *Journal of Physical Chemistry Letters*, **2017**, 8, 4113-4121	6.4	76
123	Unraveling CO adsorption on model single-atom catalysts. *Science*, **2021**, 371, 375-379	33.3	72
122	Coexistence of trapped and free excess electrons in SrTiO3. *Physical Review B*, **2015**, 91,	3.3	68
121	Structural, vibrational, and quasiparticle properties of the Peierls semiconductor BaBiO3: A hybrid functional and self-consistent GW+vertex-corrections study. *Physical Review B*, **2010**, 81,	3.3	66
120	Electronic, optical, and mechanical properties of superhard cold-compressed phases of carbon. *Applied Physics Letters*, **2011**, 99, 031901	3.4	62
119	Electronic structure of PbFe1/2Ta1/2O3: Crystallographic ordering and magnetic properties. *Physical Review B*, **2004**, 69,	3.3	60
118	Density functional study of the polar MnO(111) surface. *Physical Review B*, **2006**, 73,	3.3	59
117	Hybrid functionals applied to perovskites. *Journal of Physics Condensed Matter*, **2014**, 26, 253202	1.8	58
116	Polarons in materials. *Nature Reviews Materials*, **2021**, 6, 560-586	73.3	58
115	Polarity compensation mechanisms on the perovskite surface KTaO(001). *Science*, **2018**, 359, 572-575	33.3	57
114	Water agglomerates on FeO(001). *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E5642-E5650	11.5	57
113	Local Structure and Coordination Define Adsorption in a Model Ir /Fe O Single-Atom Catalyst. *Angewandte Chemie - International Edition*, **2019**, 58, 13961-13968	16.4	55
112	Anisotropic magnetic couplings and structure-driven canted to collinear transitions in Sr2IrO4 by magnetically constrained noncollinear DFT. *Physical Review B*, **2015**, 92,	3.3	55
111	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods. *Physical Review B*, **2011**, 84,	3.3	53
110	Formation of Mn3O4(001) on MnO(001): Surface and interface structural stability. *Physical Review B* , **2007**, 76,	3.3	53
109	Room-temperature dynamic correlation between methylammonium molecules in lead-iodine based perovskites: An ab initio molecular dynamics perspective. *Physical Review B*, **2016**, 94,	3.3	51
108	Spin fluctuation induced Weyl semimetal state in the paramagnetic phase of EuCdAs. *Science Advances*, **2019**, 5, eaaw4718	14.3	48

107	Epitaxial stabilization of MnO(111) overlayers on a Pd(100) surface. *Physical Review B*, **2007**, 75,	3.3	44
106	Donor defects and small polarons on the TiO2(110) surface. *Journal of Applied Physics*, **2016**, 119, 181503	2.5	44
105	Interplay between Adsorbates and Polarons: CO on Rutile TiO_{2}(110). *Physical Review Letters*, **2019**, 122, 016805	7.4	44
104	Formation and dynamics of small polarons on the rutile TiO2(110) surface. *Physical Review B*, **2018**, 98,	3.3	42
103	The random phase approximation applied to ice. *Journal of Chemical Physics*, **2014**, 140, 084502	3.9	40
102	Three-Dimensional Electronic Structure of the Type-II Weyl Semimetal WTe_{2}. *Physical Review Letters*, **2017**, 119, 026403	7.4	40
101	Ab initio study of the structural, electronic, and magnetic properties of MnO(100) and MnO(110). *Physical Review B*, **2007**, 75,	3.3	40
100	Structure of the c(2⨯2)-Br/Pt(110) surface. *Physical Review B*, **2002**, 65,	3.3	40
99	Influence of surface atomic structure demonstrated on oxygen incorporation mechanism at a model perovskite oxide. *Nature Communications*, **2018**, 9, 3710	17.4	40
98	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. *Journal of Physical Chemistry C*, **2017**, 121, 23045-23054	3.8	39
97	Exceptionally strong magnetism in the 4d perovskites RTcO3 (R=Ca, Sr, Ba). *Physical Review B*, **2011**, 83,	3.3	39
96	Superconducting properties of MgB2 from first principles. *Physica C: Superconductivity and Its Applications*, **2007**, 456, 45-53	1.3	37
95	Ab initio prediction of pressure-induced superconductivity in potassium. *Physical Review B*, **2006**, 73,	3.3	37
94	Structural and vibrational properties of two-dimensional MnxOy layers on Pd(100): Experiments and density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	36
93	Exceptionally large room-temperature ferroelectric polarization in the PbNiO3 multiferroic nickelate: First-principles study. *Physical Review B*, **2012**, 86,	3.3	34
92	Tuning the vertical location of helical surface states in topological insulator heterostructures via dual-proximity effects. *Scientific Reports*, **2013**, 3, 1233	4.9	34
91	Structural transitions and transport-half-metallic ferromagnetism in LaMnO3 at elevated pressure. *Physical Review B*, **2012**, 85,	3.3	33
90	Proton Ordering of Cubic Ice Ic: Spectroscopy and Computer Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 10989-10997	3.8	31

89	Two-dimensional manganese oxide nanolayers on Pd(100): the surface phase diagram. *Journal of Physics Condensed Matter*, **2009**, 21, 134008	1.8	30
88	Water Adsorption at the Tetrahedral Titania Surface Layer of SrTiO(110)-(4 □1). *Journal of Physical Chemistry C*, **2013**, 117, 26060-26069	3.8	29
87	Strain-driven onset of nontrivial topological insulating states in Zintl Sr2X compounds (X=Pb, Sn). *Physical Review B*, **2011**, 84,	3.3	29
86	Local Structure and Coordination Define Adsorption in a Model Ir1/Fe3O4 Single-Atom Catalyst. *Angewandte Chemie*, **2019**, 131, 14099-14106	3.6	28
85	Interplay between magnetic, electronic, and vibrational effects in monolayer Mn3O4 grown on Pd(100). *Journal of Chemical Physics*, **2009**, 130, 124707	3.9	28
84	Converged GW quasiparticle energies for transition metal oxide perovskites. *Physical Review Materials*, **2018**, 2,	3.2	28
83	Assessing the performance of self-consistent hybrid functional for band gap calculation in oxide semiconductors. *Journal of Physics Condensed Matter*, **2017**, 29, 454004	1.8	27
82	Lifshitz transition driven by spin fluctuations and spin-orbit renormalization in NaOsO3. *Physical Review B*, **2016**, 94,	3.3	27
81	Dimensionality-strain phase diagram of strontium iridates. *Physical Review B*, **2017**, 95,	3.3	26
80	Strained c(4 □2) CoO(1 0 0)-like monolayer on Pd(1 0 0): Experiment and theory. *Surface Science*, **2010**, 604, 529-534	1.8	26
79	Large enhancement of the photovoltaic effect in ferroelectric complex oxides through bandgap reduction. *Scientific Reports*, **2016**, 6, 28313	4.9	25
78	Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide. *Nature Communications*, **2018**, 9, 492	17.4	24
77	Lithium Niobate-Type Oxides as Visible Light Photovoltaic Materials. *Chemistry of Materials*, **2016**, 28, 25-29	9.6	24
76	Ferroelectric Oxides with Strong Visible-Light Absorption from Charge Ordering. *Chemistry of Materials*, **2017**, 29, 2445-2451	9.6	24
75	Hybrid density-functional calculation of the electronic and magnetic structures of tetragonal CuO. *Physical Review B*, **2009**, 80,	3.3	24
74	(3□)-Br/Pt(110) structure and the charge-density-wave-assisted c(2□) to (3□) phase transition. *Physical Review B*, **2004**, 69,	3.3	23
73	Relativistic GW+BSE study of the optical properties of Ruddlesden-Popper iridates. *Physical Review Materials*, **2018**, 2,	3.2	23
72	Electron and hole doping in the relativistic Mott insulator Sr2IrO4: A first-principles study using band unfolding technique. *Physical Review B*, **2016**, 94,	3.3	23

71	Polaron-Driven Surface Reconstructions. *Physical Review X*, **2017**, 7,	9.1	22
70	Halogen-induced corrosion of platinum. *Journal of the American Chemical Society*, **2009**, 131, 2827-9	16.4	20
69	Probing the geometry of copper and silver adatoms on magnetite: quantitative experiment versus theory. *Nanoscale*, **2018**, 10, 2226-2230	7.7	19
68	Anisotropy of magnetic interactions and symmetry of the order parameter in unconventional superconductor Sr2RuO4. *Npj Quantum Materials*, **2017**, 2,	5	19
67	Structural and ferroelectric transitions in magnetic nickelate PbNiO3. *New Journal of Physics*, **2014**, 16, 015030	2.9	19
66	Polymeric forms of carbon in dense lithium carbide. *Journal of Physics Condensed Matter*, **2010**, 22, 292201	1.8	18
65	Resolving the adsorption of molecular O on the rutile TiO(110) surface by noncontact atomic force microscopy. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 14827-14837	11.5	16
64	Assessing model-dielectric-dependent hybrid functionals on the antiferromagnetic transition-metal monoxides MnO, FeO, CoO, and NiO. *Journal of Physics Condensed Matter*, **2020**, 32, 015502	1.8	16
63	Energetics of the coupled electronic-structural transition in the rare-earth nickelates. *Npj Quantum Materials*, **2019**, 4,	5	15
62	Small Polarons in Transition Metal Oxides **2019**, 1-39		15
61	Combined first-principles and model Hamiltonian study of the perovskite series RMnO3 (R=La,Pr,Nd,Sm,Eu, and Gd). *Physical Review B*, **2016**, 93,	3.3	14
60	Stabilizing Single Ni Adatoms on a Two-Dimensional Porous Titania Overlayer at the SrTiO(110) Surface. *Journal of Physical Chemistry C*, **2014**, 118, 19904-19909	3.8	14
59	Structural, electronic, and ferroelectric properties of compressed CdPbO3 polymorphs. *Inorganic Chemistry*, **2013**, 52, 1032-9	5.1	14
58	Direct measurement of Ni incorporation into FeO(001). *Physical Chemistry Chemical Physics*, **2018**, 20, 16469-16476	3.6	13
57	Magnetic properties of bilayer Sr3Ir2O7: Role of epitaxial strain and oxygen vacancies. *Physical Review B*, **2017**, 95,	3.3	12
56	Structural determination and electronic properties of the 4d perovskite SrPdO3. *Physical Review B*, **2014**, 89,	3.3	12
55	Vacancy clusters at domain boundaries and band bending at the SrTiO3(110) surface. *Physical Review B*, **2014**, 90,	3.3	11
54	Phase transitions driven by competing interactions in low-dimensional systems. *Europhysics Letters*, **2010**, 92, 26004	1.6	11

53	Parametrization of LSDA+U for noncollinear magnetic configurations: Multipolar magnetism in UO2. *Physical Review Materials*, **2019**, 3,	3.2	11
52	Tunable relativistic quasiparticle electronic and excitonic behavior of the FAPb(IBr) alloy. *Physical Chemistry Chemical Physics*, **2020**, 22, 11943-11955	3.6	10
51	Strain-induced tuning of the electronic Coulomb interaction in 3d transition metal oxide perovskites. *Physical Review B*, **2018**, 98,	3.3	10
50	Chemical Pressure-Induced Ferromagnetism and Stabilization of the Metallic State in Ba1-xSrxVS3. *International Journal of Modern Physics B*, **2003**, 17, 3503-3508	1.1	10
49	Ru doping in iron-based pnictides: The □unfolded□dominant role of structural effects for superconductivity. *Physical Review B*, **2017**, 95,	3.3	9
48	Diagrammatic Monte Carlo study of Fr□lich polaron dispersion in two and three dimensions. *Physical Review B*, **2018**, 97,	3.3	9
47	Influence of Local Defects on the Dynamics of O□H Bond Breaking and Formation on a Magnetite Surface. *Journal of Physical Chemistry C*, **2019**, 123, 19742-19747	3.8	8
46	Superconductivity in SrTiO3: Dielectric Function Method for Non-Parabolic Bands. *Journal of Superconductivity and Novel Magnetism*, **2019**, 32, 2739-2744	1.5	7
45	Experimental observation of defect pair separation triggering phase transitions. *Scientific Reports*, **2014**, 4, 4110	4.9	7
44	First-principles investigation of BaFe2As2(001). *Physical Review B*, **2010**, 82,	3.3	7
43	Thickness dependent structural and electronic properties of CuO grown on SrTiO□(100): a hybrid density functional theory study. *Journal of Physics Condensed Matter*, **2011**, 23, 045004	1.8	7
42	Role of electronic correlations on the ground-state properties and on the pressure-induced metal-insulator transition in BaVS3. *Physical Review B*, **2004**, 70,	3.3	7
41	Covalent effects in magnetic ferroelectrics MnMO3 (M = Ti, Sn). *Physica Status Solidi (B): Basic Research*, **2015**, 252, 626-634	1.3	6
40	Comment on □leavage surface of the BaFe2□CoxAs2 and FeySe1□Tex superconductors: A combined STM plus LEED study□*Physical Review B*, **2012**, 86,	3.3	6
39	Electronically driven phase transitions in a quasi-one-dimensional adsorbate system. *European Physical Journal B*, **2010**, 75, 15-22	1.2	6
38	Cubic and tetragonal perovskites from the random phase approximation. *Physical Review Materials*, **2019**, 3,	3.2	6
37	CuAu, a hexagonal two-dimensional metal. *2D Materials*, **2020**, 7, 045017	5.9	5
36	Ab initio prediction of the high-pressure phase diagram of BaBiO3. *Physical Review B*, **2017**, 96,	3.3	5

35	Degenerate Phases of Iodine on Pt(110) at Half-Monolayer Coverage. *Journal of Physical Chemistry C*, **2014**, 118, 29919-29927	3.8	5
34	Tailor-made ultrathin manganese oxide nanostripes: 'magic widths' on Pd(1 1 N) terraces. *Journal of Physics Condensed Matter*, **2012**, 24, 042001	1.8	5
33	Structural, transport, and electronic properties of a layered dichalcogenide AuVS2 with semimetallic properties. *Physical Review B*, **2002**, 66,	3.3	5
32	Comparative ab initio study of the structural, electronic, magnetic, and dynamical properties of LiOsO3 and NaOsO3. *Physical Review Materials*, **2020**, 4,	3.2	5
31	Small Polarons in Transition Metal Oxides **2020**, 1035-1073		5
30	Osmates on the Verge of a Hund's-Mott Transition: The Different Fates of NaOsO_{3} and LiOsO_{3}. *Physical Review Letters*, **2020**, 125, 166402	7.4	5
29	Effective band structure of Ru-doped BaFe2As2. *Journal of Physics: Conference Series*, **2016**, 689, 012027	0.3	5
28	Halogen Phases on Pd(110): Compression Structures, Domain Walls, and Corrosion. *Journal of Physical Chemistry C*, **2015**, 119, 3613-3623	3.8	4
27	CO oxidation by Pt/FeO: Metastable dimer and support configurations facilitate lattice oxygen extraction.. *Science Advances*, **2022**, 8, eabn4580	14.3	4
26	Probing structural changes upon carbon monoxide coordination to single metal adatoms. *Journal of Chemical Physics*, **2020**, 152, 051102	3.9	3
25	Optical Response of an Interacting Polaron Gas in Strongly Polar Crystals. *Applied Sciences (Switzerland)*, **2020**, 10, 2059	2.6	3
24	Charge Trapping an Stufenkanten von Anatas-TiO2(101). *Angewandte Chemie*, **2014**, 126, 4804-4807	3.6	3
23	SrRuO3SrTiO3 heterostructure as a possible platform for studying unconventional superconductivity in Sr2RuO4. *Physical Review B*, **2020**, 101,	3.3	2
22	Kagome metal-organic frameworks as a platform for strongly correlated electrons. *JPhys Materials*, **2020**, 3, 025001	4.2	2
21	Electron-phonon interactions using the projector augmented-wave method and Wannier functions. *Physical Review B*, **2020**, 101,	3.3	2
20	Intriguing electronic and optical properties of M2CX2 (M = Mo, W; X = O, F) MXenes and their van der Waals heterostructures. *Chemical Physics Letters*, **2019**, 731, 136614	2.5	2
19	Doping-induced insulator-metal transition in the Lifshitz magnetic insulator NaOsO. *Journal of Physics Condensed Matter*, **2019**, 31, 244002	1.8	2
18	Competing magnetic interactions in a spin-12 square lattice: Hidden order in Sr2VO4. *Physical Review B*, **2017**, 96,	3.3	2

17	Chemical-pressure induced modifications on the magnetic and electronic properties of Ba 1 x Sr x VS 3. *Europhysics Letters*, **2005**, 71, 952-958	1.6	2
16	Structural and electronic properties of Hg1 MoyBa2CuO4+ *Physical Review B*, **2000**, 62, 9163-9171	3.3	2
15	Rapid oxygen exchange between hematite and water vapor. *Nature Communications*, **2021**, 12, 6488	17.4	2
14	Challenges and Opportunities in Modeling Oxides for Energy and Information Devices **2020**, 1001-1012		2
13	Electronic State Unfolding for Plane Waves: Energy Bands, Fermi Surfaces, and Spectral Functions. *Journal of Physical Chemistry C*, **2021**, 125, 12921-12928	3.8	2
12	Nanoscale synthesis of ionic analogues of bilayer silicene with high carrier mobility. *Journal of Materials Chemistry C*, **2021**, 9, 8545-8551	7.1	2
11	Doping Evolution of the Local Electronic and Structural Properties of the Double Perovskite BaNa Ca OsO. *Journal of Physical Chemistry C*, **2020**, 124, 16577-16585	3.8	1
10	Ab-initio Computation of Superconducting Properties of Elemental Superconductors and MgB2. *Journal of Superconductivity and Novel Magnetism*, **2005**, 18, 649-652		1
9	Aberrant electronic and structural alterations in pressure tuned perovskite NaOsO3. *Npj Quantum Materials*, **2020**, 5,	5	1
8	Interplay between multipolar spin interactions, Jahn-Teller effect, and electronic correlation in a Jeff=32 insulator. *Physical Review B*, **2021**, 103,	3.3	1
7	Advanced First-Principle Modeling of Relativistic Ruddlesden Popper Strontium Iridates. *Applied Sciences (Switzerland)*, **2021**, 11, 2527	2.6	1
6	Pressure-Induced Excitations in the Out-of-Plane Optical Response of the Nodal-Line Semimetal ZrSiS. *Physical Review Letters*, **2021**, 127, 076402	7.4	1
5	Ferro-octupolar Order and Low-Energy Excitations in d^{2} Double Perovskites of Osmium.. *Physical Review Letters*, **2021**, 127, 237201	7.4	0
4	Challenges and Opportunities in Modeling Oxides for Energy and Information Devices **2019**, 1-13		
3	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	0.9	
2	Special issue on novel superconducting and magnetic materials. *Journal of Physics Condensed Matter*, **2020**, 32, 040401	1.8	
1	Revealing the quasiparticle electronic and excitonic nature in cubic, tetragonal, and hexagonal phases of FAPbI3. *AIP Advances*, **2022**, 12, 025330	1.5	