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
1	Revealing the quasiparticle electronic and excitonic nature in cubic, tetragonal, and hexagonal phases of FAPbI₃. AIP Advances, 2022, 12, 025330.	0.6	2
2	Modeling polarons in density functional theory: lessons learned from TiO₂. Journal of Physics Condensed Matter, 2022, 34, 204006.	0.7	6
3	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
4	Machine learning for exploring small polaron configurational space. Npj Computational Materials, 2022, 8, .	3.5	8
5	Role of Polarons in Single-Atom Catalysts: Case Study of Me1 [Au1, Pt1, and Rh1] on TiO2(110). Topics in Catalysis, 2022, 65, 1620-1630.	1.3	3
6	Modeling magnetic multipolar phases in density functional theory. Physical Review B, 2022, 106, .	1.1	7
7	Nanoscale synthesis of ionic analogues of bilayer silicene with high carrier mobility. Journal of Materials Chemistry C, 2021, 9, 8545-8551.	2.7	4
8	Unraveling CO adsorption on model single-atom catalysts. Science, 2021, 371, 375-379.	6.0	179
9	Interplay between multipolar spin interactions, Jahn-Teller effect, and electronic correlation in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>J</mml:mi><mml:mtext>eff</mml:mtext> insulator. Physical Review B, 2021, 103, .	1.1	14
10	Polarons in materials. Nature Reviews Materials, 2021, 6, 560-586.	23.3	273
11	Advanced First-Principle Modeling of Relativistic Ruddlesdenâ€"Popper Strontium Iridates. Applied Sciences (Switzerland), 2021, 11, 2527.	1.3	5
12	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
13	Optical and excitonic properties of transition metal oxide perovskites by the Bethe-Salpeter equation. Physical Review Materials, 2021, 5, .	0.9	9
14	Pressure-Induced Excitations in the Out-of-Plane Optical Response of the Nodal-Line Semimetal ZrSiS. Physical Review Letters, 2021, 127, 076402.	2.9	6
15	Diagrammatic quantum Monte Carlo study of an acoustic lattice polaron. Physical Review B, 2021, 104, .	1.1	4
16	Ferro-octupolar Order and Low-Energy Excitations in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="normal">d</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup></mml:mrow></mml:m Perovskites of Osmium. Physical Review Letters, 2021, 127, 237201.	2.9	17
17	Rapid oxygen exchange between hematite and water vapor. Nature Communications, 2021, 12, 6488.	5.8	8
18	Special issue on novel superconducting and magnetic materials. Journal of Physics Condensed Matter, 2020, 32, 040401.	0.7	0

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19	Quantum Phases on the Verge of a Hundâ€™s-Mott Transition: The Different Fates of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NaOsO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>LiOsO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review Letters, 2020, 125, 166402.	2.9	10
20	Aberrant electronic and structural alterations in pressure tuned perovskite NaOsO3. Npj Quantum Materials, 2020, 5, .	1.8	4
21	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
22	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SrRuO</mml:mi><mml:mn>3</mml:mn></mml:m heterostructure as a possible platform for studying unconventional superconductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:m Physical Review B, 2020, 101, .	1.1	6
23	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.	0.7	30
24	Doping Evolution of the Local Electronic and Structural Properties of the Double Perovskite Ba₂Na_{1â€“x}Ca_xOsO₆. Journal of Physical Chemistry C, 2020, 124, 16577-16585.	1.5	9
25	CuAu, a hexagonal two-dimensional metal. 2D Materials, 2020, 7, 045017.	2.0	11
26	Kagome metal-organic frameworks as a platform for strongly correlated electrons. JPhys Materials, 2020, 3, 025001.	1.8	11
27	Probing structural changes upon carbon monoxide coordination to single metal adatoms. Journal of Chemical Physics, 2020, 152, 051102.	1.2	4
28	Tunable relativistic quasiparticle electronic and excitonic behavior of the FAPb(I_{1â^’x}Br_x)₃ alloy. Physical Chemistry Chemical Physics, 2020, 22, 11943-11955.	1.3	18
29	Electron-phonon interactions using the projector augmented-wave method and Wannier functions. Physical Review B, 2020, 101, .	1.1	10
30	Optical Response of an Interacting Polaron Gas in Strongly Polar Crystals. Applied Sciences (Switzerland), 2020, 10, 2059.	1.3	7
31	Small Polarons in Transition Metal Oxides. , 2020, , 1035-1073.		10
32	Comparative ab initio study of the structural, electronic, magnetic, and dynamical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiOsO</mml:mi><mml:mn>3</mml:mn></mml:msub></m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NaOsO</mml:mi><mml:mn>3</mml:mn></mml:msub></ Physical Review Materials, 2020, 4, .	0.9	11
33	Challenges and Opportunities in Modeling Oxides for Energy and Information Devices. , 2020, , 1001-1012.		2
34	Influence of Local Defects on the Dynamics of Oâ€“H Bond Breaking and Formation on a Magnetite Surface. Journal of Physical Chemistry C, 2019, 123, 19742-19747.	1.5	11
35	Spin fluctuation induced Weyl semimetal state in the paramagnetic phase of EuCd ₂ As ₂. Science Advances, 2019, 5, eaaw4718.	4.7	122
36	Local Structure and Coordination Define Adsorption in a Model Ir₁/Fe₃O₄ Singleâ€Atom Catalyst. Angewandte Chemie - International Edition, 2019, 58, 13961-13968.	7.2	93

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37	Local Structure and Coordination Define Adsorption in a Model Ir₁/Fe₃O₄ Singleâ€Atom Catalyst. Angewandte Chemie, 2019, 131, 14099-14106.	1.6	44
38	Intriguing electronic and optical properties of M2CX2 (Mâ€¯=â€¯Mo, W; Xâ€¯=â€¯O, F) MXenes and their van der Waals heterostructures. Chemical Physics Letters, 2019, 731, 136614.	1.2	13
39	Doping-induced insulator-metal transition in the Lifshitz magnetic insulator NaOsO₃. Journal of Physics Condensed Matter, 2019, 31, 244002.	0.7	3
40	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	1.9	23
41	Superconductivity in SrTiO3: Dielectric Function Method for Non-Parabolic Bands. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2739-2744.	0.8	12
42	Energetics of the coupled electronicâ€“structural transition in the rare-earth nickelates. Npj Quantum Materials, 2019, 4, .	1.8	28
43	Challenges and Opportunities in Modeling Oxides for Energy and Information Devices. , 2019, , 1-13.		0
44	Small Polarons in Transition Metal Oxides. , 2019, , 1-39.		20
45	Interplay between Adsorbates and Polarons: CO on Rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 407 Td (stretchy="false	2.9	76
46	Parametrization of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LSDA</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> for noncollinear magnetic configurations: Multipolar magnetism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>UO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review Materials, 2019, 3, .	0.9	35
47	Cubic and tetragonal perovskites from the random phase approximation. Physical Review Materials, 2019, 3, .	0.9	10
48	Defect chemistry of Eu dopants in NaI scintillators studied by atomically resolved force microscopy. Physical Review Materials, 2019, 3, .	0.9	0
49	Diagrammatic Monte Carlo study of FrÃ¶hlich polaron dispersion in two and three dimensions. Physical Review B, 2018, 97, .	1.1	26
50	Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide. Nature Communications, 2018, 9, 492.	5.8	31
51	Polarity compensation mechanisms on the perovskite surface KTaO ₃ (001). Science, 2018, 359, 572-575.	6.0	85
52	Probing the geometry of copper and silver adatoms on magnetite: quantitative experiment versus theory. Nanoscale, 2018, 10, 2226-2230.	2.8	21
53	Ab Initio study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:msub><mml:mi>BiO</mml:mi><mml:mn> (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 97 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mro	1.1	3
54	Influence of surface atomic structure demonstrated on oxygen incorporation mechanism at a model perovskite oxide. Nature Communications, 2018, 9, 3710.	5.8	54

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55	Formation and dynamics of small polarons on the rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm (110) surface. Physical Review B, 2018, 98, .	1.1	67
56	Strain-induced tuning of the electronic Coulomb interaction in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:r transition metal oxide perovskites. Physical Review B, 2018, 98, .	1.1	18
57	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
58	Direct measurement of Ni incorporation into Fe₃O₄(001). Physical Chemistry Chemical Physics, 2018, 20, 16469-16476.	1.3	20
59	Converged <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m quasiparticle energies for transition metal oxide perovskites. Physical Review Materials, 2018, 2, .	0.9	45
60	Relativistic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m +BSE study of the optical properties of Ruddlesden-Popper iridates. Physical Review Materials, 2018, 2, .	0.9	40
61	Magnetic properties of bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Sr</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Ir</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> : Role of epitaxial strain and oxygen vacancies. Physical Review B, 2017, 95, .	1.1	15
62	Dimensionality-strain phase diagram of strontium iridates. Physical Review B, 2017, 95, .	1.1	37
63	Polaron-Driven Surface Reconstructions. Physical Review X, 2017, 7, .	2.8	32
64	Ru doping in iron-based pnictides: The â€œunfoldedâ€• dominant role of structural effects for superconductivity. Physical Review B, 2017, 95, .	1.1	11
65	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. Journal of Physical Chemistry C, 2017, 121, 23045-23054.	1.5	56
66	Behavior of Methylammonium Dipoles in MAPbX₃ (X = Br and I). Journal of Physical Chemistry Letters, 2017, 8, 4113-4121.	2.1	103
67	Assessing the performance of self-consistent hybrid functional for band gap calculation in oxide semiconductors. Journal of Physics Condensed Matter, 2017, 29, 454004.	0.7	33
68	Competing magnetic interactions in a spin- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mfrac><mml:mn>1</mml:mn><mml:mn>2</mml:mn></mml:mfrac></mml square lattice: Hidden order in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:r Physical Review B, 2017, 96, .	1.1	8
69	Three-Dimensional Electronic Structure of the Type-II Weyl Semimetal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WTe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review Letters, 2017, 119, 026403.	2.9	55
70	Anisotropy of magnetic interactions and symmetry of the order parameter in unconventional superconductor Sr2RuO4. Npj Quantum Materials, 2017, 2, .	1.8	24
71	Ab initio prediction of the high-pressure phase diagram of BaBiO3. Physical Review B, 2017, 96, .	1.1	8
72	Ferroelectric Oxides with Strong Visible-Light Absorption from Charge Ordering. Chemistry of Materials, 2017, 29, 2445-2451.	3.2	32

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73	Effective band structure of Ru-doped BaFe₂As₂. Journal of Physics: Conference Series, 2016, 689, 012027.	0.3	6
74	Electron and hole doping in the relativistic Mott insulator <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Sr</mml:mi><mml:mn mathvariant="bold">2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">IrO</mml:mi><mml:mn mathvariant="bold">4</mml:mn></mml:msub></mml:mrow></mml:math> : A first-principles study using	1.1	27
75	Room-temperature dynamic correlation between methylammonium molecules in lead-iodine based perovskites: An ab initio molecular dynamics perspective. Physical Review B, 2016, 94, .	1.1	62
76	Lifshitz transition driven by spin fluctuations and spin-orbit renormalization inNaOsO3. Physical Review B, 2016, 94, .	1.1	34
77	Donor defects and small polarons on the TiO2(110) surface. Journal of Applied Physics, 2016, 119, .	1.1	51
78	Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites. Scientific Reports, 2016, 6, 28618.	1.6	234
79	Large enhancement of the photovoltaic effect in ferroelectric complex oxides through bandgap reduction. Scientific Reports, 2016, 6, 28313.	1.6	34
80	Combined first-principles and model Hamiltonian study of the perovskite series<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:mi>MnO</mml:mi></mml:mrow><mml /><mml:mn>3</mml:mn></mml:msub></mml:math><mml:math		

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91	Direct View at Excess Electrons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m and Anatase. Physical Review Letters, 2014, 113, 086402.	2.9	373
92	Vacancy clusters at domain boundaries and band bending at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">SrTiO</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mo>(</mml:mo><mml:mn>110</mml Physical Review B, 2014, 90, .	1.1	14
93	The random phase approximation applied to ice. Journal of Chemical Physics, 2014, 140, 084502.	1.2	45
94	Proton Ordering of Cubic Ice Ic: Spectroscopy and Computer Simulations. Journal of Physical Chemistry C, 2014, 118, 10989-10997.	1.5	35
95	Stabilizing Single Ni Adatoms on a Two-Dimensional Porous Titania Overlayer at the SrTiO3(110) Surface. Journal of Physical Chemistry C, 2014, 118, 19904-19909.	1.5	14
96	Hybrid functionals applied to perovskites. Journal of Physics Condensed Matter, 2014, 26, 253202.	0.7	81
97	Charge Trapping at the Step Edges of TiO₂ Anatase (101). Angewandte Chemie - International Edition, 2014, 53, 4714-4716.	7.2	102
98	Structural determination and electronic properties of the 4dperovskite SrPdO3. Physical Review B, 2014, 89, .	1.1	14
99	Experimental observation of defect pair separation triggering phase transitions. Scientific Reports, 2014, 4, 4110.	1.6	7
100	Rocksalt SnS and SnSe: Native topological crystalline insulators. Physical Review B, 2013, 88, .	1.1	104
101	Structural, Electronic, and Ferroelectric Properties of Compressed CdPbO₃ Polymorphs. Inorganic Chemistry, 2013, 52, 1032-1039.	1.9	14
102	Dual behavior of excess electrons in rutile TiO₂. Physica Status Solidi - Rapid Research Letters, 2013, 7, 199-203.	1.2	140
103	Tuning the vertical location of helical surface states in topological insulator heterostructures via dual-proximity effects. Scientific Reports, 2013, 3, 1233.	1.6	38
104	Water Adsorption at the Tetrahedral Titania Surface Layer of SrTiO₃(110)-(4 Ã— 1). Journal of Physical Chemistry C, 2013, 117, 26060-26069.	1.5	32
105	Comment on â€œCleavage surface of the BaFe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Co<m xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>As<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow	1.1	6
106	Structural transitions and transport-half-metallic ferromagnetism in LaMnO<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>at elevated pressure. Physical Review B, 2012, 85, .	1.1	36
107	Role of self-trapping in luminescence and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type conductivity of wide-band-gap oxides. Physical Review B, 2012, 85, .	1.1	440
108	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

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109	Screened hybrid functional applied to 3<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>d</mml:mi><mml:mn>0</mml:mn></mml:msup></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>â†'</mml:mo></mml:math>3<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	1.1	146
110	Maximally localized Wannier functions in LaMnO₃within PBE +U, hybrid functionals and partially self-consistent GW: an efficient route to constructab initiotight-binding parameters for e_gperovskites. Journal of Physics Condensed Matter, 2012, 24, 235602.	0.7	106
111	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
112	Tailor-made ultrathin manganese oxide nanostripes: â€˜magic widthsâ€™ on Pd(1 1N) terraces. Journal of Physics Condensed Matter, 2012, 24, 042001.	0.7	7
113	Dirac semimetal and topological phase transitions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>A</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Bi (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 572 Td (display="in	1.1	1529
114	Electronic, optical, and mechanical properties of superhard cold-compressed phases of carbon. Applied Physics Letters, 2011, 99, .	1.5	68
115	Hardness of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>T</mml:mi></mml:math>-carbon: Density functional theory calculations. Physical Review B, 2011, 84, .	1.1	140
116	Exceptionally strong magnetism in the 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"	1.1	42
117	display="inline"><mml:mrow><mml:msub><mml:m Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advancedab initiomethods. Physical Review B, 2011, 84, .	1.1	66
118	Thickness dependent structural and electronic properties of CuO grown on SrTiO₃(100): a hybrid density functional theory study. Journal of Physics Condensed Matter, 2011, 23, 045004.	0.7	8
119	Strain-driven onset of nontrivial topological insulating states in Zintl Sr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub><mml:mi>X</mml:mi></mml:mrow></mml:math>compounds		

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127	Two-dimensional manganese oxide nanolayers on Pd(100): the surface phase diagram. Journal of Physics Condensed Matter, 2009, 21, 134008.	0.7	35
128	Halogen-Induced Corrosion of Platinum. Journal of the American Chemical Society, 2009, 131, 2827-2829.	6.6	25
129	Interplay between magnetic, electronic, and vibrational effects in monolayer Mn3O4 grown on Pd(100). Journal of Chemical Physics, 2009, 130, 124707.	1.2	32
130	Hybrid density-functional calculation of the electronic and magnetic structures of tetragonal CuO. Physical Review B, 2009, 80, .	1.1	27
131	Polaronic Hole Trapping in Doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaBiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2009, 102, 256402.	2.9	93
132	Ab initiostudy of the structural, electronic, and magnetic properties ofMnO(100)andMnO(110). Physical Review B, 2007, 75, .	1.1	41
133	Formation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Mn</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mn>001</mml:mn></mml:mrow></mml:mrow></mml:math> MnO(001): Surface and interface structural stability. Physical Review B, 2007, 76, .	1.1	62
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