Jorge IÃ±iguez

List of Publications by Year
in descending order

182 papers	10,887 citations	26630 56 h-index	33894 99 g-index
188 all docs	188 docs citations	188 times ranked	10136 citing authors

#	Article	IF	Citations
1	Deterministic switching of ferromagnetism at room temperature using an electric field. Nature, 2014, 516, 370-373.	27.8	570
2	Observation of room-temperature polar skyrmions. Nature, 2019, 568, 368-372.	27.8	417
3	Exchange bias in LaNiO3â€“LaMnO3 superlattices. Nature Materials, 2012, 11, 195-198.	27.5	403
4	First-Principles Approach to Insulators in Finite Electric Fields. Physical Review Letters, 2002, 89, 117602.	7.8	387
5	A rhombohedral ferroelectric phase in epitaxially strained Hf0.5Zr0.5O2 thin films. Nature Materials, 2018, 17, 1095-1100.	27.5	324
6	Hybrid exchange-correlation functional for accurate prediction of the electronic and structural properties of ferroelectric oxides. Physical Review B, 2008, 77, .	3.2	315
7	Rare-earth nickelatesRNiO₃: thin films and heterostructures. Reports on Progress in Physics, 2018, 81, 046501.	20.1	291
8	Negative capacitance in multidomain ferroelectric superlattices. Nature, 2016, 534, 524-528.	27.8	286
9	Spatially resolved steady-state negative capacitance. Nature, 2019, 565, 468-471.	27.8	245
10	Molecular and dissociative adsorption of multiple hydrogen molecules on transition metal decoratedC60. Physical Review B, 2005, 72, .	3.2	234
11	First-principles predictions of low-energy phases of multiferroic BiFeO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2011, 83, .	3.2	216
12	Ferroelectric negative capacitance. Nature Reviews Materials, 2019, 4, 243-256.	48.7	179
13	First-principles study of(BiScO3)1â^'xâ^'(PbTiO3)xpiezoelectric alloys. Physical Review B, 2003, 67, .	3.2	161
14	Raman spectroscopy of rare-earth orthoferrites <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mi>FeO</mml:mi><mml:m (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>R</mml:mi></mml:math>) Tj ETQq0 0 0 rgBT /Overlock 1	3.2	159
15	Phase coexistence and electric-field control of toroidal order in oxide superlattices. Nature Materials, 2017, 16, 1003-1009.	27.5	159
16	Near room-temperature multiferroic materials with tunable ferromagnetic and electrical properties. Nature Communications, 2014, 5, 4021.	12.8	152
17	Designing lead-free antiferroelectrics for energy storage. Nature Communications, 2017, 8, 15682.	12.8	149
18	Artificial chemical and magnetic structure at the domain walls of an epitaxial oxide. Nature, 2014, 515, 379-383.	27.8	146

#	Article	IF	Citations
19	Spin-phonon coupling effects in transition-metal perovskites: A DFTÂ+Â<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>and hybrid-functional study. Physical Review B, 2012, 85, .	3.2	145
20	Structure and hydrogen dynamics of pure and Ti-doped sodium alanate. Physical Review B, 2004, 70, .	3.2	144
21	Orbital and Spin Chains inZnV2O4. Physical Review Letters, 2004, 93, 156407.	7.8	144
22	Structurally triggered metal-insulator transition in rare-earth nickelates. Nature Communications, 2017, 8, 1677.	12.8	122
23	Emergent chirality in the electric polarization texture of titanate superlattices. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 915-920.	7.1	121
24	Optical control of polarization in ferroelectric heterostructures. Nature Communications, 2018, 9, 3344.	12.8	119
25	Complete phase diagram of rare-earth nickelates from first-principles. Npj Quantum Materials, 2017, 2, .	5.2	113
26	Second-principles method for materials simulations including electron and lattice degrees of freedom. Physical Review B, 2016, 93, .	3.2	112
27	First-Principles Study of the Temperature-Pressure Phase Diagram ofBaTiO3. Physical Review Letters, 2002, 89, 115503.	7.8	106
28	A Single-Component Molecular Metal Based on a Thiazole Dithiolate Gold Complex. Journal of the American Chemical Society, 2009, 131, 16961-16967.	13.7	102
29	Novel Nanoscale Twinned Phases in Perovskite Oxides. Advanced Functional Materials, 2013, 23, 234-240.	14.9	101
30	AbÂInitioIndications for Giant Magnetoelectric Effects Driven by Structural Softness. Physical Review Letters, 2010, 105, 037208.	7.8	99
31	Dynamics of Berry-phase polarization in time-dependent electric fields. Physical Review B, 2004, 69, .	3.2	98
32	First-Principles Approach to Lattice-Mediated Magnetoelectric Effects. Physical Review Letters, 2008, 101, 117201.	7.8	91
33	First-principles model potentials for lattice-dynamical studies: general methodology and example of application to ferroic perovskite oxides. Journal of Physics Condensed Matter, 2013, 25, 305401.	1.8	90
34	CaFeO₂: A New Type of Layered Structure with Iron in a Distorted Square Planar Coordination. Journal of the American Chemical Society, 2009, 131, 221-229.	13.7	89
35	Multiferroic Phase Transition near Room Temperature in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Films. Physical Review Letters, 2011, 107, 237601.	7.8	88
36	Ferroelectric Transitions at Ferroelectric Domain Walls Found from First Principles. Physical Review Letters, 2014, 112, 247603.	7.8	88

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37	Magnetoelectric Response of Multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>and Related Materials from First-Principles Calculations. Physical Review Letters, 2009, 103, 267205.	7.8	87
38	Anomalous properties in ferroelectrics induced by atomic ordering. Nature, 2001, 413, 54-57.	27.8	86
39	Local negative permittivity and topological phase transition in polar skyrmions. Nature Materials, 2021, 20, 194-201.	27.5	86
40	First-Principles Investigation of Morphotropic Transitions and Phase-Change Functional Responses in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi>BiCoO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Mult Solid Solutions. Physical Review Letters, 2011, 107, 057601.	7.8	85
41	Universal collaborative couplings between oxygen-octahedral rotations and antiferroelectric distortions in perovskites. Physical Review B, 2013, 88, .	3.2	83
42	Magnetic Cycloid of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>from Atomistic Simulations. Physical Review Letters, 2012, 109, 037207.	7.8	82
43	Finiteâ€Temperature Properties of Rareâ€Earthâ€Substituted BiFeO₃ Multiferroic Solid Solutions. Advanced Functional Materials, 2015, 25, 552-558.	14.9	78
44	Tuning the atomic and domain structure of epitaxial films of multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BiFeO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m Physical Review B, 2010, 81, .	3.2	77
45	Anisotropic Chemical Pressure Effects in Single-Component Molecular Metals Based on Radical Dithiolene and Diselenolene Gold Complexes. Journal of the American Chemical Society, 2012, 134, 17138-17148.	13.7	73
46	First-principles study of the multimode antiferroelectric transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">PbZrO</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	3.2	73
47	Prediction of a native ferroelectric metal. Nature Communications, 2016, 7, 11211.	12.8	71
48	Domain walls in a perovskite oxide with two primary structural order parameters: First-principles study of BiFeO<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>. Physical Review B, 2013, 87, .	3.2	69
49	Microscopic origins of the large piezoelectricity of leadfree (Ba,Ca)(Zr,Ti)O3. Nature Communications, 2017, 8, 15944.	12.8	69
50	Structural and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrFeO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m first principles. Physical Review B, 2008, 78, .	3.2	68
51	Electric control of the magnetization in BiFeO<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>/LaFeO<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, .	3.2	63
52	Conductivity and Local Structure of LaNiO₃ Thin Films. Advanced Materials, 2017, 29, 1605197.	21.0	63
53	First-principles study of Ti-doped sodium alanate surfaces. Applied Physics Letters, 2005, 86, 103109.	3.3	60
54	Origin of the magnetization and compensation temperature in rare-earth orthoferrites and orthochromates. Physical Review B, 2016, 93, .	3.2	59

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55	Theoretical guidelines to create and tune electric skyrmion bubbles. Science Advances, 2019, 5, eaau7023.	10.3	59
56	First-principles investigation of the structural phases and enhanced response properties of the BiFeO<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>-LaFeO<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>multiferroic solid solution. Physical Review B, 2012,	3.2	58
57	Atomistic simulations of the incipient ferroelectricKTaO3. Physical Review B, 2004, 70, .	3.2	56
58	Ab initiostudy of proper topological ferroelectricity in layered perovskite La<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>	3.2	56
59	Prediction of a Novel Magnetoelectric Switching Mechanism in Multiferroics. Physical Review Letters, 2014, 112, 057202.	7.8	55
60	Ferroelectric Domains in Multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Films under Epitaxial Strains. Physical Review Letters, 2013, 110, 187601.	7.8	54
61	Multiple strain-induced phase transitions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LaNi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>thin films. Physical Review B, 2016, 94, .	3.2	54
62	Pressure-induced structural, electronic, and magnetic effects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BiFeO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m Physical Review B, 2009, 79, .	3.2	53
63	Improper electric polarization in simple perovskite oxides with two magnetic sublattices. Nature Communications, 2017, 8, 14025.	12.8	53
64	Atomistic theory of hybrid improper ferroelectricity in perovskites. Physical Review B, 2014, 89, .	3.2	51
65	Devonshire-Landau free energy ofBaTiO3from first principles. Physical Review B, 2001, 63, .	3.2	50
66	Insights into the phase diagram of bismuth ferrite from quasiharmonic free-energy calculations. Physical Review B, 2013, 88, .	3.2	50
67	Hybrid Improper Ferroelectricity in Multiferroic Superlattices: Finiteâ€Temperature Properties and Electricâ€Fieldâ€Driven Switching of Polarization and Magnetization. Advanced Functional Materials, 2015, 25, 3626-3633.	14.9	49
68	Ab Initio Design of Perovskite Alloys with Predetermined Properties: The Case ofPb(Sc0.5Nb0.5)O3. Physical Review Letters, 2001, 87, 095503.	7.8	48
69	Quantitative analysis of the first-principles effective Hamiltonian approach to ferroelectric perovskites. Physical Review B, 2003, 67, .	3.2	48
70	Electroresistance Effect in Ferroelectric Tunnel Junctions with Symmetric Electrodes. ACS Nano, 2012, 6, 1473-1478.	14.6	48
71	Stable Metallic State of a Neutral-Radical Single-Component Conductor at Ambient Pressure. Journal of the American Chemical Society, 2018, 140, 6998-7004.	13.7	48
72	Amorphization Induced by Pressure: Results for Zeolites and General Implications. Physical Review Letters, 2006, 97, 225502.	7.8	47

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73	Rules and mechanisms governing octahedral tilts in perovskites under pressure. Physical Review B, 2017, 96, .	3.2	45
74	Deterministic and robust room-temperature exchange coupling in monodomain multiferroic BiFeO3 heterostructures. Nature Communications, 2017, 8, 1583.	12.8	45
75	Ultrafast Switching of the Electric Polarization and Magnetic Chirality in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>BiFeO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn> an Electric Field. Physical Review Letters, 2014, 112, 147601.	7.8	44
76	Ultralow Voltage Manipulation of Ferromagnetism. Advanced Materials, 2020, 32, e2001943.	21.0	44
77	Cooperative Couplings between Octahedral Rotations and Ferroelectricity in Perovskites and Related Materials. Physical Review Letters, 2018, 120, 197602.	7.8	43
78	Multiple structural transitions driven by spin-phonon couplings in a perovskite oxide. Science Advances, 2017, 3, e1700288.	10.3	42
79	Manipulating magnetoelectric energy landscape in multiferroics. Nature Communications, 2020, 11, 2836.	12.8	42
80	Photoinduced Phase Transitions in Ferroelectrics. Physical Review Letters, 2019, 123, 087601.	7.8	40
81	A phononic switch based on ferroelectric domain walls. Physical Review B, 2017, 96, .	3.2	39
82	Meta-screening and permanence of polar distortion in metallized ferroelectrics. Physical Review B, 2018, 97, .	3.2	39
83	Piezoelectricity in hafnia. Nature Communications, 2021, 12, 7301.	12.8	37
84	Strain Engineering Magnetic Frustration in Perovskite Oxide Thin Films. Physical Review Letters, 2012, 109, 247202.	7.8	36
85	First-Principles Simulations on the Nature of the Melting Line of Sodium. Physical Review Letters, 2007, 98, 055501.	7.8	35
86	Ferroelectricity with Asymmetric Hysteresis in Metallic <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:mn> Ultrathin Films. Physical Review Letters, 2019, 122, 227601.	7.8	34
87	Energetics of oxygen-octahedra rotations in perovskite oxides from first principles. Physical Review B, 2018, 97, .	3.2	32
88	Tuning the Weak Ferromagnetic States in Dysprosium Orthoferrite. Scientific Reports, 2016, 6, 37529.	3.3	31
89	Electric-Field Control of Magnetization, Jahn-Teller Distortion, and Orbital Ordering in Ferroelectric Ferromagnets. Physical Review Letters, 2019, 122, 247701.	7.8	31
90	Direct observation of ferroelectricity in two-dimensional MoS2. Npj 2D Materials and Applications, 2022, 6, .	7.9	30

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91	Epitaxial phases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>BiMnO</mml:mtext><mml:mn>3</mml:mn></mml:msub></mml:math> first principles. Physical Review B, 2015, 91, .	3.2	27
92	Ferroelectric domain wall phonon polarizer. Physical Review Materials, 2017, 1, .	2.4	27
93	Pressureâ€Induced Multiferroics via Pseudo Jahnâ€“Teller Effects and Novel Couplings. Advanced Functional Materials, 2017, 27, 1604513.	14.9	25
94	Electric control of the heat flux through electrophononic effects. Physical Review B, 2018, 97, .	3.2	25
95	The role of lattice dynamics in ferroelectric switching. Nature Communications, 2022, 13, 1110.	12.8	25
96	Effects of Atomic Short-Range Order on the Properties of Perovskite Alloys in their Morphotropic Phase Boundary. Physical Review Letters, 2003, 91, 045504.	7.8	24
97	Effects of vacancies on the properties of disordered ferroelectrics: A first-principles study. Physical Review B, 2007, 75, .	3.2	24
98	Improper ferroelectricity at antiferromagnetic domain walls of perovskite oxides. Physical Review B, 2017, 96, .	3.2	24
99	Electrocaloric effects in the lead-free Ba(Zr,Ti)O3 relaxor ferroelectric from atomistic simulations. Physical Review B, 2017, 96, .	3.2	24
100	Giant electrocaloric response in the prototypical Pb(Mg,Nb) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> relaxor ferroelectric from atomistic simulations. Physical Review B, 2018, 97, .	3.2	24
101	Optical phonons associated with the low-temperature ferroelectric properties of perovskite solid solutions. Physical Review B, 2002, 65, .	3.2	23
102	Efficient systematic scheme to construct second-principles lattice dynamical models. Physical Review B, 2017, 95, .	3.2	23
103	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	4.0	23
104	Probing Antiferroelectricâ€Ferroelectric Phase Transitions in PbZrO₃ Capacitors by Piezoresponse Force Microscopy. Advanced Functional Materials, 2020, 30, 2003622.	14.9	23
105	Wake-up Free Ferroelectric Rhombohedral Phase in Epitaxially Strained ZrO₂ Thin Films. ACS Applied Materials & Interfaces, 2021, 13, 51383-51392.	8.0	23
106	Electrical phase diagram of bulk<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review B, 2015, 92, .	3.2	22
107	Single-Component Conductors: A Sturdy Electronic Structure Generated by Bulky Substituents. Inorganic Chemistry, 2016, 55, 6036-6046.	4.0	22
108	Giant direct and inverse electrocaloric effects in multiferroic thin films. Physical Review B, 2018, 98, .	3.2	22

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109	Atomistic mechanism leading to complex antiferroelectric and incommensurate perovskites. Physical Review B, 2016, 94, .	3.2	21
110	First-Principles Study of Ferroelastic Twins in Halide Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 1416-1421.	4.6	21
111	Flat branches and pressure amorphization. Journal of Non-Crystalline Solids, 2002, 307-310, 602-612.	3.1	20
112	Theoretical phase diagram of ultrathin films of incipient ferroelectrics. Applied Physics Letters, 2007, 90, 242918.	3.3	20
113	First-principles study of a pressure-induced spin transition in multiferroic Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>FeCrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	3.2	20
114	Testing simple predictors for the temperature of a structural phase transition. Physical Review B, 2014, 90, .	3.2	20
115	On the possibility that PbZrO3 not be antiferroelectric. Npj Computational Materials, 2021, 7, .	8.7	20
116	Symmetry breaking at the nanoscale and diffuse transitions in ferroelectrics: A comparative study ofPbSc1â^•2Nb1â^•2O3andPbZr0.6Ti0.4O3. Physical Review B, 2006, 73, .	3.2	19
117	Archetypal Soft-Mode-Driven Antipolar Transition in Francisite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Cu</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:msub><mml:mrow><mml:mi>SeO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mrow /><mml:mrow /></mml:msub><mml:mo stretchy="false">)</mml:mo></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2020, 124, 097603.	7.8	19
118	Self-averaging of random and thermally disordered diluted Ising systems. Physical Review E, 1999, 60, 2394-2397.	2.1	18
119	Ab initiostudy of the factors affecting the ground state of rare-earth nickelates. Physical Review B, 2012, 85, .	3.2	18
120	Deterministic control of ferroelectric polarization by ultrafast laser pulses. Nature Communications, 2022, 13, 2566.	12.8	18
121	Universality class of thermally diluted Ising systems at criticality. Physical Review E, 2000, 62, 191-196.	2.1	16
122	Neutral and Charged Oxygen Vacancies Induce Two-Dimensional Electron Gas Near SiO₂/BaTiO₃ Interfaces. Journal of Physical Chemistry Letters, 2013, 4, 333-337.	4.6	16
123	Complex domain walls in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2015, 91, .	3.2	16
124	Vibrational properties of TiHn complexes adsorbed on carbon nanostructures. Chemical Physics Letters, 2007, 444, 140-144.	2.6	15
125	Fermi Resonance Involving Nonlinear Dynamical Couplings in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Pb</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi>Zr</mml:mi><mml:mo>,</mml:mo><mml:mi>Ti</mml:mi><mml:mo) Tj ETQq1 1 0.784314 rgBT mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Solid Solutions. Physical Review Letters, 2011, 107, 175502.	7.8	15
126	Elucidation of crystal and electronic structures within highly strained BiFeO3 by transmission electron microscopy and first-principles simulation. Scientific Reports, 2017, 7, 46498.	3.3	15

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127	Tailoring properties of hybrid perovskites by domain-width engineering with charged walls. Npj Computational Materials, 2018, 4, .	8.7	15
128	Effect of Dopant Ordering on the Stability of Ferroelectric Hafnia. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000047.	2.4	15
129	Raman Imaging Approach to the Study of Ferroelectric Domains and Raman Spectra of Multiferroic Boracites. Acta Physica Polonica A, 2009, 116, 19-24.	0.5	15
130	Theoretical investigation of hydrogen storage in metal-intercalated graphitic materials. Journal of Physics Condensed Matter, 2008, 20, 285212.	1.8	14
131	Interplay between elasticity, ferroelectricity and magnetism at the domain walls of bismuth ferrite. Physica Status Solidi - Rapid Research Letters, 2016, 10, 209-217.	2.4	14
132	Quantum-fluctuation-stabilized orthorhombic ferroelectric ground state in lead-free piezoelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mi>Ba</mml:mi><mml:m mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 98, .	3.2	14
133	Thermal conductivity changes across a structural phase transition: The case of high-pressure silica. Physical Review B, 2017, 96, .	3.2	13
134	A key piece of the ferroelectric hafnia puzzle. Science, 2020, 369, 1300-1301.	12.6	13
135	Vibrational properties of LaNiO3 films in the ultrathin regime. APL Materials, 2020, 8, .	5.1	13
136	Strain engineering of ZnO thermal conductivity. Physical Review Materials, 2019, 3, .	2.4	13
137	Giant Thermal Transport Tuning at a Metal/Ferroelectric Interface. Advanced Materials, 2022, 34, e2105778.	21.0	13
138	Giant Electrophononic Response in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>PbTiO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mn><mml:m by Strain Engineering. Physical Review Letters, 2019, 123, 185901.	7.8	12
139	Theoretical investigation of lattice thermal conductivity and electrophononic effects in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi Physical Review Materials, 2019, 3, .	2.4	12
140	THERMALLY DILUTED ISING SYSTEMS. Fractals, 2003, 11, 53-65.	3.7	11
141	Anomalous properties of antiferroelectric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>PbZrO</mml:mtext><mml:mn>3</mml:mn></mml:msub></mml:math> hydrostatic pressure. Physical Review B, 2014, 89, .	3.2	11
142	Magnetic phase diagram of rare-earth orthorhombic perovskite oxides. Physical Review B, 2021, 104, .	3.2	11
143	Optimized local modes for lattice-dynamical applications. Physical Review B, 2000, 61, 3127-3130.	3.2	10
144	Polymorphism in Bi-based perovskite oxides: A first-principles study. Physical Review Materials, 2018, 2, .	2.4	10

#	Article	IF	Citations
145	Phonons and magnetoelectric interactions in Ni3V2O8. Journal of Physics Condensed Matter, 2008, 20, 434214.	1.8	9
146	An efficient computational method for use in structural studies of crystals with substitutional disorder. Journal of Physics Condensed Matter, 2010, 22, 415401.	1.8	9
147	Phase diagram of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:msub><mml:mi mathvariant="normal">LaFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>superlattices studied by x-ray diffraction experiments and first-principles calculations. Physical Review B, 2014, 90, .	3.2	9
148	Multiferroic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:m mathvariant="normal">NiMnO</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:math> thin films: A computational prediction. Physical Review B, 2017, 95, .	3.2	9
149	Unusual structural tuning of magnetism in cuprate perovskites. Physical Review B, 2005, 71, .	3.2	8
150	Hydrogen-related catalytic effects of Ti and other light transition metals on NaAlH4surfaces. Journal of Physics Condensed Matter, 2007, 19, 176007.	1.8	8
151	Magnetoelectric effects via pentalinear interactions. Physical Review B, 2015, 92, .	3.2	8
152	High-pressure structural change in the ferroelectric layered perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">S</mml:mi><mml:msub><mml:mi mathvariant="normal">r</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant	3.2	8
153	Anisotropy-driven thermal conductivity switching and thermal hysteresis in a ferroelectric. Applied Physics Letters, 2019, 115, 192903.	3.3	8
154	A three-order-parameter bistable magnetoelectric multiferroic metal. Nature Communications, 2020, 11, 4922.	12.8	8
155	Novel type of ferroelectricity in brownmillerite structures: A first-principles study. Physical Review Materials, 2018, 2, .	2.4	8
156	A unified perturbative approach to electrocaloric effects. Communications Materials, 2021, 2, .	6.9	7
157	Analysis of soft optical modes in hexagonal BaTiO3: transference of perovskite local distortions. Journal of Physics Condensed Matter, 2000, 12, L387-L391.	1.8	6
158	Temperature-Dependent Classical Phonons from Efficient Nondynamical Simulations. Physical Review Letters, 2013, 110, 105503.	7.8	6
159	Strategy to utilize transmission electron microscopy and X-ray diffraction to investigate biaxial strain effect in epitaxial BiFeO₃ films. Japanese Journal of Applied Physics, 2018, 57, 0902A5.	1.5	6
160	Origin of nonlinear magnetoelectric response in rare-earth orthoferrite perovskite oxides. Physical Review B, 2022, 105, .	3.2	6
161	Chiral structures of electric polarization vectors quantified by X-ray resonant scattering. Nature Communications, 2022, 13, 1769.	12.8	6
162	Magnetoelectric signature in the magnetic properties of antiferromagnetic multiferroics: Atomistic simulations and phenomenology. Physical Review B, 2013, 88, .	3.2	5

#	Article	IF	Citations
163	Structural and magnetic transitions accompanied by large responses in epitaxial Sr0.5Ba0.5MnO3 films. Physical Review Materials, 2018, 2, .	2.4	5
164	Pressure amorphization through displacive disorder. European Physical Journal E, 2002, 9, 239-243.	1.6	4
165	Creating multiferroic and conductive domain walls in common ferroelastic compounds. Npj Computational Materials, 2019, 5, .	8.7	4
166	Electrocaloric effects in multiferroics. Physical Review B, 2021, 103, .	3.2	4
167	Phonons in the cubic phase of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	Article	IF	Citations
181	Probing Strain-Induced Phenomena in Low Dimensionality Multiferroic Oxides. Microscopy and Microanalysis, 2017, 23, 1726-1727.	0.4	0
182	First-principles screening of ABO3 oxides with two magnetic sublattices. Physical Review Materials, 2019, 3, .	2.4	0