

# Jorge Iñiguez

## List of Publications by Year in descending order

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182  
papers

10,887  
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26630

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188  
docs citations

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times ranked

10136  
citing authors

#	ARTICLE	IF	CITATIONS
1	Energetic Couplings in Ferroics. <i>Advanced Electronic Materials</i> , 2022, 8, 2100639.	5.1	3
2	Giant Thermal Transport Tuning at a Metal/Ferroelectric Interface. <i>Advanced Materials</i> , 2022, 34, e2105778.	21.0	13
3	Origin of nonlinear magnetoelectric response in rare-earth orthoferrite perovskite oxides. <i>Physical Review B</i> , 2022, 105, .	3.2	6
4	Electrical Energy Storage From First Principles. <i>Frontiers in Electronic Materials</i> , 2022, 2, .	3.1	3
5	The role of lattice dynamics in ferroelectric switching. <i>Nature Communications</i> , 2022, 13, 1110.	12.8	25
6	Direct observation of ferroelectricity in two-dimensional MoS <sub>2</sub> . <i>Npj 2D Materials and Applications</i> , 2022, 6, .	7.9	30
7	Chiral structures of electric polarization vectors quantified by X-ray resonant scattering. <i>Nature Communications</i> , 2022, 13, 1769.	12.8	6
8	Deterministic control of ferroelectric polarization by ultrafast laser pulses. <i>Nature Communications</i> , 2022, 13, 2566.	12.8	18
9	Local negative permittivity and topological phase transition in polar skyrmions. <i>Nature Materials</i> , 2021, 20, 194-201.	27.5	86
10	Structural and Raman study of the thermoelectric solid solution Sr <sub>1.9</sub> La <sub>0.1</sub> Nb <sub>2</sub> O <sub>7</sub> . <i>Journal of Raman Spectroscopy</i> , 2021, 52, 737-749.	2.5	1
11	Electrocaloric effects in multiferroics. <i>Physical Review B</i> , 2021, 103, .	3.2	4
12	A unified perturbative approach to electrocaloric effects. <i>Communications Materials</i> , 2021, 2, .	6.9	7
13	Magnetic phase diagram of rare-earth orthorhombic perovskite oxides. <i>Physical Review B</i> , 2021, 104, .	3.2	11
14	Wake-up Free Ferroelectric Rhombohedral Phase in Epitaxially Strained ZrO <sub>2</sub> Thin Films. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 51383-51392.	8.0	23
15	Coexisting conventional and inverse mechanocaloric effects in ferroelectrics. <i>Physical Review B</i> , 2021, 104, .	3.2	1
16	Piezoelectricity in hafnia. <i>Nature Communications</i> , 2021, 12, 7301.	12.8	37
17	On the possibility that PbZrO <sub>3</sub> not be antiferroelectric. <i>Npj Computational Materials</i> , 2021, 7, .	8.7	20
18	A three-order-parameter bistable magnetoelectric multiferroic metal. <i>Nature Communications</i> , 2020, 11, 4922.	12.8	8

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19	Antiferroelectricity in a family of pyroxene-like oxides with rich polymorphism. Communications Materials, 2020, 1, .	6.9	2
20	Probing Antiferroelectric-Ferroelectric Phase Transitions in $\text{PbZrO}_3$ Capacitors by Piezoresponse Force Microscopy. Advanced Functional Materials, 2020, 30, 2003622.	14.9	23
21	A key piece of the ferroelectric hafnia puzzle. Science, 2020, 369, 1300-1301.	12.6	13
22	Ultralow Voltage Manipulation of Ferromagnetism. Advanced Materials, 2020, 32, e2001943.	21.0	44
23	Vibrational properties of $\text{LaNiO}_3$ films in the ultrathin regime. APL Materials, 2020, 8, .	5.1	13
24	Manipulating magnetoelectric energy landscape in multiferroics. Nature Communications, 2020, 11, 2836. <i>Archetypal Soft-Mode-Driven Antipolar Transition in Francisite</i>	12.8	42
25	<i>Physical Review Letters, 2020, 124, 097603.</i> Archetypal Soft-Mode-Driven Antipolar Transition in Francisite $\langle \text{Cu} \rangle$	7.8	19
26	Effect of Dopant Ordering on the Stability of Ferroelectric Hafnia. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000047.	2.4	15
27	First-Principles Studies of Structural Domain Walls. , 2020, , 36-75.		3
28	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	4.0	23
29	Giant Electrophononic Response in $\text{PbTiO}_3$ High-Pressure Structural Change in the Ferroelectric Layered Perovskite $\text{SrS}_{2-r}\text{N}_b$	7.8	19
30	$\text{SrS}_{2-r}\text{N}_b$	3.2	8
31	Photoinduced Phase Transitions in Ferroelectrics. Physical Review Letters, 2019, 123, 087601.	7.8	40
32	Creating multiferroic and conductive domain walls in common ferroelastic compounds. Npj Computational Materials, 2019, 5, .	8.7	4
33	Electric-Field Control of Magnetization, Jahn-Teller Distortion, and Orbital Ordering in Ferroelectric Ferromagnets. Physical Review Letters, 2019, 122, 247701.	7.8	31
34	Ferroelectricity with Asymmetric Hysteresis in Metallic $\text{LiOsO}_4$ Ultrathin Films. Physical Review Letters, 2019, 122, 227601.	7.8	34
35	Observation of room-temperature polar skyrmions. Nature, 2019, 568, 368-372.	27.8	417
36	First-Principles Study of Ferroelastic Twins in Halide Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 1416-1421.	4.6	21

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37	Ferroelectric negative capacitance. Nature Reviews Materials, 2019, 4, 243-256.	48.7	179
38	Theoretical guidelines to create and tune electric skyrmion bubbles. Science Advances, 2019, 5, eaau7023.	10.3	59
39	Anisotropy-driven thermal conductivity switching and thermal hysteresis in a ferroelectric. Applied Physics Letters, 2019, 115, 192903.	3.3	8
40	Spatially resolved steady-state negative capacitance. Nature, 2019, 565, 468-471.	27.8	245
41	Theoretical investigation of lattice thermal conductivity and electrophononic effects in $\text{SrTiO}_3$ . Physical Review Materials, 2019, 3, .	2.4	12
42	Strain engineering of ZnO thermal conductivity. Physical Review Materials, 2019, 3, .	2.4	13
43	First-principles screening of ABO <sub>3</sub> oxides with two magnetic sublattices. Physical Review Materials, 2019, 3, .	2.4	0
44	Meta-screening and permanence of polar distortion in metallized ferroelectrics. Physical Review B, 2018, 97, .	3.2	39
45	Energetics of oxygen-octahedra rotations in perovskite oxides from first principles. Physical Review B, 2018, 97, .	3.2	32
46	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
47	Rare-earth nickelates $\text{RNiO}_3$ : thin films and heterostructures. Reports on Progress in Physics, 2018, 81, 046501.	20.1	291
48	Giant electrocaloric response in the prototypical $\text{Pb}(\text{Mg,Nb})\text{O}_3$ relaxor ferroelectric from atomistic simulations. Physical Review B, 2018, 97, .	3.2	24
49	Giant direct and inverse electrocaloric effects in multiferroic thin films. Physical Review B, 2018, 98, .	3.2	22
50	Tailoring properties of hybrid perovskites by domain-width engineering with charged walls. Npj Computational Materials, 2018, 4, .	8.7	15
51	A rhombohedral ferroelectric phase in epitaxially strained $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$ thin films. Nature Materials, 2018, 17, 1095-1100.	27.5	324
52	Strategy to utilize transmission electron microscopy and X-ray diffraction to investigate biaxial strain effect in epitaxial $\text{BiFeO}_3$ films. Japanese Journal of Applied Physics, 2018, 57, 0902A5.	1.5	6
53	Quantum-fluctuation-stabilized orthorhombic ferroelectric ground state in lead-free piezoelectric $\text{BaTiO}_3$ . Physical Review B, 2018, 98, .	3.2	11
54	Electric control of the heat flux through electrophononic effects. Physical Review B, 2018, 97, .	3.2	25

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55	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
56	Cooperative Couplings between Octahedral Rotations and Ferroelectricity in Perovskites and Related Materials. Physical Review Letters, 2018, 120, 197602.	7.8	43
57	Optical control of polarization in ferroelectric heterostructures. Nature Communications, 2018, 9, 3344.	12.8	119
58	Novel type of ferroelectricity in brownmillerite structures: A first-principles study. Physical Review Materials, 2018, 2, .	2.4	8
59	Structural and magnetic transitions accompanied by large responses in epitaxial Sr0.5Ba0.5MnO3 films. Physical Review Materials, 2018, 2, .	2.4	5
60	Polymorphism in Bi-based perovskite oxides: A first-principles study. Physical Review Materials, 2018, 2, .	2.4	10
61	Improper electric polarization in simple perovskite oxides with two magnetic sublattices. Nature Communications, 2017, 8, 14025.	12.8	53
62	Conductivity and Local Structure of LaNiO <sub>3</sub> Thin Films. Advanced Materials, 2017, 29, 1605197.	21.0	63
63	Elucidation of crystal and electronic structures within highly strained BiFeO <sub>3</sub> by transmission electron microscopy and first-principles simulation. Scientific Reports, 2017, 7, 46498.	3.3	15
64	Complete phase diagram of rare-earth nickelates from first-principles. Npj Quantum Materials, 2017, 2, .	5.2	113
65	Designing lead-free antiferroelectrics for energy storage. Nature Communications, 2017, 8, 15682.	12.8	149
66	Multiferroic $\text{Bi}_2\text{NiMnO}_6$ thin films: A computational prediction. Physical Review B, 2017, 95, .	3.2	9
67	Efficient systematic scheme to construct second-principles lattice dynamical models. Physical Review B, 2017, 95, .	3.2	23
68	Pressure-Induced Multiferroics via Pseudo Jahn-Teller Effects and Novel Couplings. Advanced Functional Materials, 2017, 27, 1604513.	14.9	25
69	Multiple structural transitions driven by spin-phonon couplings in a perovskite oxide. Science Advances, 2017, 3, e1700288.	10.3	42
70	Improper ferroelectricity at antiferromagnetic domain walls of perovskite oxides. Physical Review B, 2017, 96, .	3.2	24
71	Electrocaloric effects in the lead-free Ba(Zr,Ti)O <sub>3</sub> relaxor ferroelectric from atomistic simulations. Physical Review B, 2017, 96, .	3.2	24
72	Rules and mechanisms governing octahedral tilts in perovskites under pressure. Physical Review B, 2017, 96, .	3.2	45

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73	Phase coexistence and electric-field control of toroidal order in oxide superlattices. Nature Materials, 2017, 16, 1003-1009.	27.5	159
74	Probing Strain-Induced Phenomena in Low Dimensionality Multiferroic Oxides. Microscopy and Microanalysis, 2017, 23, 1726-1727.	0.4	0
75	Deterministic and robust room-temperature exchange coupling in monodomain multiferroic BiFeO <sub>3</sub> heterostructures. Nature Communications, 2017, 8, 1583.	12.8	45
76	Structurally triggered metal-insulator transition in rare-earth nickelates. Nature Communications, 2017, 8, 1677.	12.8	122
77	Thermal conductivity changes across a structural phase transition: The case of high-pressure silica. Physical Review B, 2017, 96, .	3.2	13
78	A phononic switch based on ferroelectric domain walls. Physical Review B, 2017, 96, .	3.2	39
79	Microscopic origins of the large piezoelectricity of leadfree (Ba,Ca)(Zr,Ti)O <sub>3</sub> . Nature Communications, 2017, 8, 15944.	12.8	69
80	Ferroelectric domain wall phonon polarizer. Physical Review Materials, 2017, 1, .	2.4	27
81	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
82	Tuning the Weak Ferromagnetic States in Dysprosium Orthoferrite. Scientific Reports, 2016, 6, 37529.	3.3	31
83	Raman spectroscopy of rare-earth orthoferrites $R\text{FeO}_3$ ( $R = \text{La, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu}$ ) Tj ETQq1 10.784314 rgBT / DV		
84	Multiple strain-induced phase transitions in $\text{LaNiO}_3$ thin films. Physical Review B, 2016, 94, .	3.2	54
85	Atomistic mechanism leading to complex antiferroelectric and incommensurate perovskites. Physical Review B, 2016, 94, .	3.2	21
86	Second-principles method for materials simulations including electron and lattice degrees of freedom. Physical Review B, 2016, 93, .	3.2	112
87	Origin of the magnetization and compensation temperature in rare-earth orthoferrites and orthochromates. Physical Review B, 2016, 93, .	3.2	59
88	Prediction of a native ferroelectric metal. Nature Communications, 2016, 7, 11211.	12.8	71
89	Single-Component Conductors: A Sturdy Electronic Structure Generated by Bulky Substituents. Inorganic Chemistry, 2016, 55, 6036-6046.	4.0	22
90	Negative capacitance in multidomain ferroelectric superlattices. Nature, 2016, 534, 524-528.	27.8	286

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91	Exploiting interfacial and size effects to construct oxide superlattices with robust and tunable magnetoelectric properties at room temperature. <i>Physical Review B</i> , 2015, 91, .	3.2	3
92	Magnetoelectric effects via pentalinear interactions. <i>Physical Review B</i> , 2015, 92, .	3.2	8
93	Electrical phase diagram of bulk $\text{BiFeO}_3$ . <i>Physical Review B</i> , 2015, 92, .	3.2	20
94	Hybrid Improper Ferroelectricity in Multiferroic Superlattices: Finite-Temperature Properties and Electric-Field-Driven Switching of Polarization and Magnetization. <i>Advanced Functional Materials</i> , 2015, 25, 3626-3633.	14.9	49
95	Complex domain walls in $\text{BiFeO}_3$ . <i>Physical Review B</i> , 2015, 91, .	3.2	6
96	Epitaxial phases of $\text{BiMnO}_3$ and first principles. <i>Physical Review B</i> , 2015, 91, .	3.2	27
97	E-MRS Fall Meeting, Technical University of Warsaw, September 2014, Symposium "Functional Perovskite Systems". <i>Phase Transitions</i> , 2015, 88, 951-952.	1.3	0
98	Finite-Temperature Properties of Rare-Earth-Substituted $\text{BiFeO}_3$ Multiferroic Solid Solutions. <i>Advanced Functional Materials</i> , 2015, 25, 552-558.	14.9	78
99	Deterministic switching of ferromagnetism at room temperature using an electric field. <i>Nature</i> , 2014, 516, 370-373.	27.8	570
100	Publisher's Note: Phase diagram of $\text{BiFeO}_3$ studied by x-ray diffraction experiments and first-principles calculations [ <i>Phys. Rev. B</i> 90, 104106 (2014)]. <i>Physical Review B</i> , 2014, 90, .	3.2	1
101	First-principles study of the multimode antiferroelectric transition in $\text{PbZrO}_3$ . <i>Physical Review B</i> , 2014, 90, .	3.2	73
102	Ultrafast Switching of the Electric Polarization and Magnetic Chirality in $\text{BiFeO}_3$ an Electric Field. <i>Physical Review Letters</i> , 2014, 112, 147601.	7.8	14
103	Near room-temperature multiferroic materials with tunable ferromagnetic and electrical properties. <i>Nature Communications</i> , 2014, 5, 4021.	12.8	152
104	Atomistic theory of hybrid improper ferroelectricity in perovskites. <i>Physical Review B</i> , 2014, 89, .	3.2	51
105	Prediction of a Novel Magnetoelectric Switching Mechanism in Multiferroics. <i>Physical Review Letters</i> , 2014, 112, 057202.	7.8	55
106	Artificial chemical and magnetic structure at the domain walls of an epitaxial oxide. <i>Nature</i> , 2014, 515, 379-383.	27.8	146
107	Testing simple predictors for the temperature of a structural phase transition. <i>Physical Review B</i> , 2014, 90, .	3.2	20
108	Phase diagram of $\text{BiFeO}_3/\text{LaFeO}_3$ superlattices studied by x-ray diffraction experiments and first-principles calculations. <i>Physical Review B</i> , 2014, 90, .	3.2	9



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109	Anomalous properties of antiferroelectric $\text{PbZrO}_3$ under hydrostatic pressure. <i>Physical Review B</i> , 2014, 89, .	11.1	11
110	Ferroelectric Transitions at Ferroelectric Domain Walls Found from First Principles. <i>Physical Review Letters</i> , 2014, 112, 247603.	7.8	88
111	Universal collaborative couplings between oxygen-octahedral rotations and antiferroelectric distortions in perovskites. <i>Physical Review B</i> , 2013, 88, .	3.2	83
112	Neutral and Charged Oxygen Vacancies Induce Two-Dimensional Electron Gas Near $\text{SiO}_2/\text{BaTiO}_3$ Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 333-337.	4.6	16
113	Electric control of the magnetization in $\text{BiFeO}_3/\text{LaFeO}_3$ superlattices. <i>Physical Review B</i> , 2013, 88, .	3.2	63
114	Insights into the phase diagram of bismuth ferrite from quasiharmonic free-energy calculations. <i>Physical Review B</i> , 2013, 88, .	3.2	50
115	Magnetoelectric signature in the magnetic properties of antiferromagnetic multiferroics: Atomistic simulations and phenomenology. <i>Physical Review B</i> , 2013, 88, .	3.2	5
116	Ferroelectric Domains in Multiferroic $\text{BiFeO}_3$ Films under Epitaxial Strains. <i>Physical Review Letters</i> , 2013, 110, 187601.	7.8	54
117	Domain walls in a perovskite oxide with two primary structural order parameters: First-principles study of $\text{BiFeO}_3$ . <i>Physical Review B</i> , 2013, 87, .	3.2	69
118	First-principles model potentials for lattice-dynamical studies: general methodology and example of application to ferroic perovskite oxides. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 305401.	1.8	90
119	Novel Nanoscale Twinned Phases in Perovskite Oxides. <i>Advanced Functional Materials</i> , 2013, 23, 234-240.	14.9	101
120	Temperature-Dependent Classical Phonons from Efficient Nondynamical Simulations. <i>Physical Review Letters</i> , 2013, 110, 105503.	7.8	6
121	<i>Ab initio</i> study of the factors affecting the ground state of rare-earth nickelates. <i>Physical Review B</i> , 2012, 85, .	3.2	18
122	Anisotropic Chemical Pressure Effects in Single-Component Molecular Metals Based on Radical Dithiolene and Diselenolene Gold Complexes. <i>Journal of the American Chemical Society</i> , 2012, 134, 17138-17148.	13.7	73
123	Electroresistance Effect in Ferroelectric Tunnel Junctions with Symmetric Electrodes. <i>ACS Nano</i> , 2012, 6, 1473-1478.	14.6	48
124	First-principles investigation of the structural phases and enhanced response properties of the $\text{BiFeO}_3/\text{LaFeO}_3$ multiferroic solid solution. <i>Physical Review B</i> , 2012, .	3.2	58
125	Exchange bias in $\text{LaNiO}_3/\text{LaMnO}_3$ superlattices. <i>Nature Materials</i> , 2012, 11, 195-198.	27.5	403
126	Spin-phonon coupling effects in transition-metal perovskites: A DFT+ $\hat{U}$ and hybrid-functional study. <i>Physical Review B</i> , 2012, 85, .	3.2	145



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127	Magnetic Cycloid of $\text{BiFeO}_3$ from Atomistic Simulations. <i>Physical Review Letters</i> , 2012, 109, 037207.	7.8	82
128	First-principles study of a pressure-induced spin transition in multiferroic $\text{BiFeO}_3$ . <i>Physical Review Letters</i> , 2011, 107, 237601.	3.2	20
129	Strain Engineering Magnetic Frustration in Perovskite Oxide Thin Films. <i>Physical Review Letters</i> , 2012, 109, 247202.	7.8	36
130	Multiferroic Phase Transition near Room Temperature in $\text{BiFeO}_3$ Films. <i>Physical Review Letters</i> , 2011, 107, 237601.	7.8	88
131	First-principles investigation of Morphotropic Transitions and Phase-Change Functional Responses in $\text{TiO}_2$ . <i>Physical Review Letters</i> , 2011, 107, 057601.	3.2	56
132	First-Principles Investigation of Morphotropic Transitions and Phase-Change Functional Responses in $\text{BiFeO}_3$ . <i>Physical Review Letters</i> , 2011, 107, 057601.	7.8	85
133	First-principles predictions of low-energy phases of multiferroic $\text{BiFeO}_3$ . <i>Physical Review Letters</i> , 2011, 107, 057601.	3.2	216
134	Fermi Resonance Involving Nonlinear Dynamical Couplings in $\text{PbTiO}_3$ Solid Solutions. <i>Physical Review Letters</i> , 2011, 107, 057601.	7.8	15
135	Tuning the atomic and domain structure of epitaxial films of multiferroic $\text{BiFeO}_3$ . <i>Physical Review B</i> , 2010, 81, .	3.2	77
136	An efficient computational method for use in structural studies of crystals with substitutional disorder. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 415401.	1.8	9
137	<i>Ab Initio</i> Indications for Giant Magnetoelectric Effects Driven by Structural Softness. <i>Physical Review Letters</i> , 2010, 105, 037208.	7.8	99
138	Pressure-induced structural, electronic, and magnetic effects in $\text{BiFeO}_3$ . <i>Physical Review B</i> , 2009, 79, .	3.2	53
139	A Single-Component Molecular Metal Based on a Thiazole Dithiolate Gold Complex. <i>Journal of the American Chemical Society</i> , 2009, 131, 16961-16967.	13.7	102
140	Magnetoelectric Response of Multiferroic $\text{BiFeO}_3$ and Related Materials from First-Principles Calculations. <i>Physical Review Letters</i> , 2009, 103, 267205.	7.8	87
141	Phonons in the cubic phase of $\text{BiFeO}_3$ .		

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145	Modelling of carbon-based materials for hydrogen storage. , 2008, , 205-220.		1
146	Phonons and magnetoelectric interactions in Ni <sub>3</sub> V <sub>2</sub> O <sub>8</sub> . Journal of Physics Condensed Matter, 2008, 20, 434214.	1.8	9
147	Theoretical investigation of hydrogen storage in metal-intercalated graphitic materials. Journal of Physics Condensed Matter, 2008, 20, 285212.	1.8	14
148	Structural and electronic properties of $\text{SrFeO}_{2.2}$ first principles. Physical Review B, 2008, 78, .	3.2	68
149	First-Principles Approach to Lattice-Mediated Magnetoelectric Effects. Physical Review Letters, 2008, 101, 117201.	7.8	91
150	Hydrogen-related catalytic effects of Ti and other light transition metals on NaAlH <sub>4</sub> surfaces. Journal of Physics Condensed Matter, 2007, 19, 176007.	1.8	8
151	Theoretical phase diagram of ultrathin films of incipient ferroelectrics. Applied Physics Letters, 2007, 90, 242918.	3.3	20
152	First-Principles Simulations on the Nature of the Melting Line of Sodium. Physical Review Letters, 2007, 98, 055501.	7.8	35
153	Effects of vacancies on the properties of disordered ferroelectrics: A first-principles study. Physical Review B, 2007, 75, .	3.2	24
154	Vibrational properties of TiH <sub>n</sub> complexes adsorbed on carbon nanostructures. Chemical Physics Letters, 2007, 444, 140-144.	2.6	15
155	Amorphization Induced by Pressure: Results for Zeolites and General Implications. Physical Review Letters, 2006, 97, 225502.	7.8	47
156	Symmetry breaking at the nanoscale and diffuse transitions in ferroelectrics: A comparative study of PbSc <sub>1-x</sub> Nb <sub>x</sub> O <sub>3</sub> and PbZr <sub>0.6</sub> Ti <sub>0.4</sub> O <sub>3</sub> . Physical Review B, 2006, 73, .	3.2	19
157	Molecular and dissociative adsorption of multiple hydrogen molecules on transition metal decorated C <sub>60</sub> . Physical Review B, 2005, 72, .	3.2	234
158	Unusual structural tuning of magnetism in cuprate perovskites. Physical Review B, 2005, 71, .	3.2	8
159	First-principles study of Ti-doped sodium alanate surfaces. Applied Physics Letters, 2005, 86, 103109.	3.3	60
160	Atomistic simulations of the incipient ferroelectric KTaO <sub>3</sub> . Physical Review B, 2004, 70, .	3.2	56
161	Structure and hydrogen dynamics of pure and Ti-doped sodium alanate. Physical Review B, 2004, 70, .	3.2	144
162	Dynamics of Berry-phase polarization in time-dependent electric fields. Physical Review B, 2004, 69, .	3.2	98

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163	Orbital and Spin Chains in ZnV <sub>2</sub> O <sub>4</sub> . Physical Review Letters, 2004, 93, 156407.	7.8	144
164	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
165	First-principles study of (BiScO <sub>3</sub> ) <sub>1-x</sub> (PbTiO <sub>3</sub> ) <sub>x</sub> piezoelectric alloys. Physical Review B, 2003, 67, .	3.2	161
166	Quantitative analysis of the first-principles effective Hamiltonian approach to ferroelectric perovskites. Physical Review B, 2003, 67, .	3.2	48
167	THERMALLY DILUTED ISING SYSTEMS. Fractals, 2003, 11, 53-65.	3.7	11
168	Optical phonons associated with the low-temperature ferroelectric properties of perovskite solid solutions. Physical Review B, 2002, 65, .	3.2	23
169	First-Principles Study of the Temperature-Pressure Phase Diagram of BaTiO <sub>3</sub> . Physical Review Letters, 2002, 89, 115503.	7.8	106
170	First-Principles Approach to Insulators in Finite Electric Fields. Physical Review Letters, 2002, 89, 117602.	7.8	387
171	Flat branches and pressure amorphization. Journal of Non-Crystalline Solids, 2002, 307-310, 602-612.	3.1	20
172	Effective-Hamiltonian Modeling of External Pressures in Ferroelectric Perovskites. AIP Conference Proceedings, 2002, , .	0.4	0
173	Pressure amorphization through displacive disorder. European Physical Journal E, 2002, 9, 239-243.	1.6	4
174	Devonshire-Landau free energy of BaTiO <sub>3</sub> from first principles. Physical Review B, 2001, 63, .	3.2	50
175	Anomalous properties in ferroelectrics induced by atomic ordering. Nature, 2001, 413, 54-57.	27.8	86
176	Ab Initio Design of Perovskite Alloys with Predetermined Properties: The Case of Pb(Sc <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub> . Physical Review Letters, 2001, 87, 095503.	7.8	48
177	Local mode transferability from cubic perovskite to hexagonal barium titanate. AIP Conference Proceedings, 2000, , .	0.4	0
178	Universality class of thermally diluted Ising systems at criticality. Physical Review E, 2000, 62, 191-196.	2.1	16
179	Optimized local modes for lattice-dynamical applications. Physical Review B, 2000, 61, 3127-3130.	3.2	10
180	First-principles study of the structural instabilities in hexagonal barium titanate: Coupling between the soft optical and the acoustic Modes. Ferroelectrics, 2000, 237, 25-32.	0.6	2

#	ARTICLE	IF	CITATIONS
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