

Jorge Iiguez

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

171
papers

8,099
citations

51
h-index

85
g-index

188
ext. papers

9,586
ext. citations

9
avg, IF

6.34
L-index

#	Paper	IF	Citations
171	The role of lattice dynamics in ferroelectric switching.. <i>Nature Communications</i> , 2022 , 13, 1110	17.4	6
170	Chiral structures of electric polarization vectors quantified by X-ray resonant scattering.. <i>Nature Communications</i> , 2022 , 13, 1769	17.4	0
169	Deterministic control of ferroelectric polarization by ultrafast laser pulses.. <i>Nature Communications</i> , 2022 , 13, 2566	17.4	1
168	Piezoelectricity in hafnia.. <i>Nature Communications</i> , 2021 , 12, 7301	17.4	4
167	Wake-up Free Ferroelectric Rhombohedral Phase in Epitaxially Strained ZrO Thin Films. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 51383-51392	9.5	6
166	Giant Thermal Transport Tuning at a Metal/Ferroelectric Interface. <i>Advanced Materials</i> , 2021 , e2105778	24	2
165	Local negative permittivity and topological phase transition in polar skyrmions. <i>Nature Materials</i> , 2021 , 20, 194-201	27	33
164	Structural and Raman study of the thermoelectric solid solution Sr _{1.9} La _{0.1} Nb ₂ O ₇ . <i>Journal of Raman Spectroscopy</i> , 2021 , 52, 737-749	2.3	0
163	Magnetic phase diagram of rare-earth orthorhombic perovskite oxides. <i>Physical Review B</i> , 2021 , 104,	3.3	2
162	Ultralow Voltage Manipulation of Ferromagnetism. <i>Advanced Materials</i> , 2020 , 32, e2001943	24	21
161	Vibrational properties of LaNiO ₃ films in the ultrathin regime. <i>APL Materials</i> , 2020 , 8, 061102	5.7	5
160	Manipulating magnetoelectric energy landscape in multiferroics. <i>Nature Communications</i> , 2020 , 11, 2836	17.4	18
159	Archetypal Soft-Mode-Driven Antipolar Transition in Francisite Cu ₃ Bi(SeO ₃) ₂ O ₂ Cl. <i>Physical Review Letters</i> , 2020 , 124, 097603	7.4	9
158	Effect of Dopant Ordering on the Stability of Ferroelectric Hafnia. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020 , 14, 2000047	2.5	7
157	A three-order-parameter bistable magnetoelectric multiferroic metal. <i>Nature Communications</i> , 2020 , 11, 4922	17.4	4
156	Antiferroelectricity in a family of pyroxene-like oxides with rich polymorphism. <i>Communications Materials</i> , 2020 , 1,	6	1
155	Probing Antiferroelectric-Ferroelectric Phase Transitions in PbZrO ₃ Capacitors by Piezoresponse Force Microscopy. <i>Advanced Functional Materials</i> , 2020 , 30, 2003622	15.6	11

154	A key piece of the ferroelectric hafnia puzzle. <i>Science</i> , 2020 , 369, 1300-1301	33.3	10
153	High-pressure structural change in the ferroelectric layered perovskite Sr ₂ Nb ₂ O ₇ . <i>Physical Review B</i> , 2019 , 100,	3.3	4
152	Photoinduced Phase Transitions in Ferroelectrics. <i>Physical Review Letters</i> , 2019 , 123, 087601	7.4	17
151	Creating multiferroic and conductive domain walls in common ferroelastic compounds. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	2
150	Electric-Field Control of Magnetization, Jahn-Teller Distortion, and Orbital Ordering in Ferroelectric Ferromagnets. <i>Physical Review Letters</i> , 2019 , 122, 247701	7.4	15
149	Ferroelectricity with Asymmetric Hysteresis in Metallic LiOsO ₃ Ultrathin Films. <i>Physical Review Letters</i> , 2019 , 122, 227601	7.4	20
148	Observation of room-temperature polar skyrmions. <i>Nature</i> , 2019 , 568, 368-372	50.4	221
147	First-Principles Study of Ferroelastic Twins in Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 1416-1421	6.4	18
146	Ferroelectric negative capacitance. <i>Nature Reviews Materials</i> , 2019 , 4, 243-256	73.3	106
145	Giant Electrophononic Response in PbTiO ₃ by Strain Engineering. <i>Physical Review Letters</i> , 2019 , 123, 185901	7.4	5
144	Theoretical investigation of lattice thermal conductivity and electrophononic effects in SrTiO ₃ . <i>Physical Review Materials</i> , 2019 , 3,	3.2	7
143	Strain engineering of ZnO thermal conductivity. <i>Physical Review Materials</i> , 2019 , 3,	3.2	9
142	Theoretical guidelines to create and tune electric skyrmion bubbles. <i>Science Advances</i> , 2019 , 5, eaau7023	14.3	27
141	Anisotropy-driven thermal conductivity switching and thermal hysteresis in a ferroelectric. <i>Applied Physics Letters</i> , 2019 , 115, 192903	3.4	3
140	Spatially resolved steady-state negative capacitance. <i>Nature</i> , 2019 , 565, 468-471	50.4	144
139	Meta-screening and permanence of polar distortion in metallized ferroelectrics. <i>Physical Review B</i> , 2018 , 97,	3.3	24
138	Energetics of oxygen-octahedra rotations in perovskite oxides from first principles. <i>Physical Review B</i> , 2018 , 97,	3.3	19
137	Emergent chirality in the electric polarization texture of titanate superlattices. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 915-920	11.5	73

136	Rare-earth nickelates RNiO: thin films and heterostructures. <i>Reports on Progress in Physics</i> , 2018 , 81, 046501	14.4	170
135	Giant electrocaloric response in the prototypical Pb(Mg,Nb)O ₃ relaxor ferroelectric from atomistic simulations. <i>Physical Review B</i> , 2018 , 97,	3.3	12
134	Stable Metallic State of a Neutral-Radical Single-Component Conductor at Ambient Pressure. <i>Journal of the American Chemical Society</i> , 2018 , 140, 6998-7004	16.4	35
133	Cooperative Couplings between Octahedral Rotations and Ferroelectricity in Perovskites and Related Materials. <i>Physical Review Letters</i> , 2018 , 120, 197602	7.4	29
132	Optical control of polarization in ferroelectric heterostructures. <i>Nature Communications</i> , 2018 , 9, 3344	17.4	69
131	Novel type of ferroelectricity in brownmillerite structures: A first-principles study. <i>Physical Review Materials</i> , 2018 , 2,	3.2	4
130	Structural and magnetic transitions accompanied by large responses in epitaxial Sr _{0.5} Ba _{0.5} MnO ₃ films. <i>Physical Review Materials</i> , 2018 , 2,	3.2	4
129	Polymorphism in Bi-based perovskite oxides: A first-principles study. <i>Physical Review Materials</i> , 2018 , 2,	3.2	7
128	Giant direct and inverse electrocaloric effects in multiferroic thin films. <i>Physical Review B</i> , 2018 , 98,	3.3	16
127	Tailoring properties of hybrid perovskites by domain-width engineering with charged walls. <i>Npj Computational Materials</i> , 2018 , 4,	10.9	12
126	A rhombohedral ferroelectric phase in epitaxially strained HfZrO thin films. <i>Nature Materials</i> , 2018 , 17, 1095-1100	27	196
125	Strategy to utilize transmission electron microscopy and X-ray diffraction to investigate biaxial strain effect in epitaxial BiFeO ₃ films. <i>Japanese Journal of Applied Physics</i> , 2018 , 57, 0902A5	1.4	4
124	Quantum-fluctuation-stabilized orthorhombic ferroelectric ground state in lead-free piezoelectric (Ba,Ca)(Zr,Ti)O ₃ . <i>Physical Review B</i> , 2018 , 98,	3.3	7
123	Electric control of the heat flux through electrophononic effects. <i>Physical Review B</i> , 2018 , 97,	3.3	17
122	Improper electric polarization in simple perovskite oxides with two magnetic sublattices. <i>Nature Communications</i> , 2017 , 8, 14025	17.4	36
121	Conductivity and Local Structure of LaNiO Thin Films. <i>Advanced Materials</i> , 2017 , 29, 1605197	24	36
120	Elucidation of crystal and electronic structures within highly strained BiFeO by transmission electron microscopy and first-principles simulation. <i>Scientific Reports</i> , 2017 , 7, 46498	4.9	11
119	Complete phase diagram of rare-earth nickelates from first-principles. <i>Npj Quantum Materials</i> , 2017 , 2,	5	77

118	Designing lead-free antiferroelectrics for energy storage. <i>Nature Communications</i> , 2017 , 8, 15682	17.4	107
117	Multiferroic Bi ₂ NiMnO ₆ thin films: A computational prediction. <i>Physical Review B</i> , 2017 , 95,	3.3	6
116	Efficient systematic scheme to construct second-principles lattice dynamical models. <i>Physical Review B</i> , 2017 , 95,	3.3	15
115	Pressure-Induced Multiferroics via Pseudo Jahn-Teller Effects and Novel Couplings. <i>Advanced Functional Materials</i> , 2017 , 27, 1604513	15.6	22
114	Multiple structural transitions driven by spin-phonon couplings in a perovskite oxide. <i>Science Advances</i> , 2017 , 3, e1700288	14.3	29
113	Improper ferroelectricity at antiferromagnetic domain walls of perovskite oxides. <i>Physical Review B</i> , 2017 , 96,	3.3	19
112	Electrocaloric effects in the lead-free Ba(Zr,Ti)O ₃ relaxor ferroelectric from atomistic simulations. <i>Physical Review B</i> , 2017 , 96,	3.3	14
111	Rules and mechanisms governing octahedral tilts in perovskites under pressure. <i>Physical Review B</i> , 2017 , 96,	3.3	29
110	Phase coexistence and electric-field control of toroidal order in oxide superlattices. <i>Nature Materials</i> , 2017 , 16, 1003-1009	27	108
109	Probing Strain-Induced Phenomena in Low Dimensionality Multiferroic Oxides. <i>Microscopy and Microanalysis</i> , 2017 , 23, 1726-1727	0.5	
108	Deterministic and robust room-temperature exchange coupling in monodomain multiferroic BiFeO ₃ heterostructures. <i>Nature Communications</i> , 2017 , 8, 1583	17.4	35
107	Structurally triggered metal-insulator transition in rare-earth nickelates. <i>Nature Communications</i> , 2017 , 8, 1677	17.4	77
106	Thermal conductivity changes across a structural phase transition: The case of high-pressure silica. <i>Physical Review B</i> , 2017 , 96,	3.3	9
105	A phononic switch based on ferroelectric domain walls. <i>Physical Review B</i> , 2017 , 96,	3.3	25
104	Microscopic origins of the large piezoelectricity of leadfree (Ba,Ca)(Zr,Ti)O ₃ . <i>Nature Communications</i> , 2017 , 8, 15944	17.4	54
103	Ferroelectric domain wall phonon polarizer. <i>Physical Review Materials</i> , 2017 , 1,	3.2	21
102	Atomistic mechanism leading to complex antiferroelectric and incommensurate perovskites. <i>Physical Review B</i> , 2016 , 94,	3.3	10
101	Second-principles method for materials simulations including electron and lattice degrees of freedom. <i>Physical Review B</i> , 2016 , 93,	3.3	83

100	Origin of the magnetization and compensation temperature in rare-earth orthoferrites and orthochromates. <i>Physical Review B</i> , 2016 , 93,	3.3	43
99	Prediction of a native ferroelectric metal. <i>Nature Communications</i> , 2016 , 7, 11211	17.4	48
98	Single-Component Conductors: A Sturdy Electronic Structure Generated by Bulky Substituents. <i>Inorganic Chemistry</i> , 2016 , 55, 6036-46	5.1	18
97	Negative capacitance in multidomain ferroelectric superlattices. <i>Nature</i> , 2016 , 534, 524-8	50.4	205
96	Valence states of new Mn coordination sites at the ferromagnetic domain walls of TbMnO ₃ thin films 2016 , 750-751		
95	Interplay between elasticity, ferroelectricity and magnetism at the domain walls of bismuth ferrite. <i>Physica Status Solidi - Rapid Research Letters</i> , 2016 , 10, 209-217	2.5	13
94	Tuning the Weak Ferromagnetic States in Dysprosium Orthoferrite. <i>Scientific Reports</i> , 2016 , 6, 37529	4.9	19
93	Raman spectroscopy of rare-earth orthoferrites RFeO ₃ (R=La, Sm, Eu, Gd, Tb, Dy). <i>Physical Review B</i> , 2016 , 94,	3.3	102
92	Multiple strain-induced phase transitions in LaNiO ₃ thin films. <i>Physical Review B</i> , 2016 , 94,	3.3	38
91	Complex domain walls in BiFeO ₃ . <i>Physical Review B</i> , 2015 , 91,	3.3	14
90	Epitaxial phases of BiMnO ₃ from first principles. <i>Physical Review B</i> , 2015 , 91,	3.3	20
89	E-MRS Fall Meeting, Technical University of Warsaw, September 2014, Symposium Functional Perovskite Systems <i>Phase Transitions</i> , 2015 , 88, 951-952	1.3	
88	Finite-Temperature Properties of Rare-Earth-Substituted BiFeO ₃ Multiferroic Solid Solutions. <i>Advanced Functional Materials</i> , 2015 , 25, 552-558	15.6	55
87	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,	3.3	3
86	Magnetoelectric effects via pentalinear interactions. <i>Physical Review B</i> , 2015 , 92,	3.3	5
85	Electrical phase diagram of bulk BiFeO ₃ . <i>Physical Review B</i> , 2015 , 92,	3.3	19
84	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	15.6	37
83	Ultrafast switching of the electric polarization and magnetic chirality in BiFeO ₃ by an electric field. <i>Physical Review Letters</i> , 2014 , 112, 147601	7.4	34

82	Near room-temperature multiferroic materials with tunable ferromagnetic and electrical properties. <i>Nature Communications</i> , 2014 , 5, 4021	17.4	127
81	Atomistic theory of hybrid improper ferroelectricity in perovskites. <i>Physical Review B</i> , 2014 , 89,	3.3	40
80	Prediction of a novel magnetoelectric switching mechanism in multiferroics. <i>Physical Review Letters</i> , 2014 , 112, 057202	7.4	51
79	Artificial chemical and magnetic structure at the domain walls of an epitaxial oxide. <i>Nature</i> , 2014 , 515, 379-83	50.4	128
78	Testing simple predictors for the temperature of a structural phase transition. <i>Physical Review B</i> , 2014 , 90,	3.3	17
77	Phase diagram of BiFeO ₃ /LaFeO ₃ superlattices studied by x-ray diffraction experiments and first-principles calculations. <i>Physical Review B</i> , 2014 , 90,	3.3	9
76	Anomalous properties of antiferroelectric PbZrO ₃ under hydrostatic pressure. <i>Physical Review B</i> , 2014 , 89,	3.3	7
75	Ferroelectric transitions at ferroelectric domain walls found from first principles. <i>Physical Review Letters</i> , 2014 , 112, 247603	7.4	63
74	Deterministic switching of ferromagnetism at room temperature using an electric field. <i>Nature</i> , 2014 , 516, 370-3	50.4	449
73	First-principles study of the multimode antiferroelectric transition in PbZrO ₃ . <i>Physical Review B</i> , 2014 , 90,	3.3	47
72	Universal collaborative couplings between oxygen-octahedral rotations and antiferroelectric distortions in perovskites. <i>Physical Review B</i> , 2013 , 88,	3.3	67
71	Neutral and Charged Oxygen Vacancies Induce Two-Dimensional Electron Gas Near SiO ₂ /BaTiO ₃ Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 333-7	6.4	14
70	Electric control of the magnetization in BiFeO ₃ /LaFeO ₃ superlattices. <i>Physical Review B</i> , 2013 , 88,	3.3	54
69	Insights into the phase diagram of bismuth ferrite from quasiharmonic free-energy calculations. <i>Physical Review B</i> , 2013 , 88,	3.3	46
68	Magnetoelectric signature in the magnetic properties of antiferromagnetic multiferroics: Atomistic simulations and phenomenology. <i>Physical Review B</i> , 2013 , 88,	3.3	5
67	Ferroelectric domains in multiferroic BiFeO ₃ films under epitaxial strains. <i>Physical Review Letters</i> , 2013 , 110, 187601	7.4	52
66	Domain walls in a perovskite oxide with two primary structural order parameters: First-principles study of BiFeO ₃ . <i>Physical Review B</i> , 2013 , 87,	3.3	59
65	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	60

64	Novel Nanoscale Twinned Phases in Perovskite Oxides. <i>Advanced Functional Materials</i> , 2013 , 23, 234-240	5.6	81
63	Temperature-dependent classical phonons from efficient nondynamical simulations. <i>Physical Review Letters</i> , 2013 , 110, 105503	7.4	6
62	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, 17138-48	16.4	65
61	Electroresistance effect in ferroelectric tunnel junctions with symmetric electrodes. <i>ACS Nano</i> , 2012 , 6, 1473-8	16.7	42
60	First-principles investigation of the structural phases and enhanced response properties of the BiFeO ₃ -LaFeO ₃ multiferroic solid solution. <i>Physical Review B</i> , 2012 , 85,	3.3	50
59	Exchange bias in LaNiO ₃ -LaMnO ₃ superlattices. <i>Nature Materials</i> , 2012 , 11, 195-8	27	358
58	Spin-phonon coupling effects in transition-metal perovskites: A DFT + U and hybrid-functional study. <i>Physical Review B</i> , 2012 , 85,	3.3	126
57	Magnetic cycloid of BiFeO ₃ from atomistic simulations. <i>Physical Review Letters</i> , 2012 , 109, 037207	7.4	67
56	First-principles study of a pressure-induced spin transition in multiferroic Bi ₂ FeCrO ₆ . <i>Physical Review B</i> , 2012 , 86,	3.3	18
55	Strain engineering magnetic frustration in perovskite oxide thin films. <i>Physical Review Letters</i> , 2012 , 109, 247202	7.4	30
54	Ab initio study of the factors affecting the ground state of rare-earth nickelates. <i>Physical Review B</i> , 2012 , 85,	3.3	16
53	Multiferroic phase transition near room temperature in BiFeO ₃ films. <i>Physical Review Letters</i> , 2011 , 107, 237601	7.4	80
52	Ab initio study of proper topological ferroelectricity in layered perovskite La ₂ Ti ₂ O ₇ . <i>Physical Review B</i> , 2011 , 84,	3.3	42
51	First-principles investigation of morphotropic transitions and phase-change functional responses in BiFeO ₃ -BiCoO ₃ multiferroic solid solutions. <i>Physical Review Letters</i> , 2011 , 107, 057601	7.4	73
50	First-principles predictions of low-energy phases of multiferroic BiFeO ₃ . <i>Physical Review B</i> , 2011 , 83,	3.3	191
49	Fermi resonance involving nonlinear dynamical couplings in Pb(Zr,Ti)O ₃ solid solutions. <i>Physical Review Letters</i> , 2011 , 107, 175502	7.4	13
48	Tuning the atomic and domain structure of epitaxial films of multiferroic BiFeO ₃ . <i>Physical Review B</i> , 2010 , 81,	3.3	68
47	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	6

46	Ab-initio indications for giant magnetoelectric effects driven by structural softness. <i>Physical Review Letters</i> , 2010 , 105, 037208	7.4	90
45	Pressure-induced structural, electronic, and magnetic effects in BiFeO ₃ . <i>Physical Review B</i> , 2009 , 79,	3.3	48
44	A single-component molecular metal based on a thiazole dithiolate gold complex. <i>Journal of the American Chemical Society</i> , 2009 , 131, 16961-7	16.4	92
43	Magnetoelectric response of multiferroic BiFeO ₃ and related materials from first-principles calculations. <i>Physical Review Letters</i> , 2009 , 103, 267205	7.4	80
42	Phonons in the cubic phase of Co ₃ B ₇ O ₁₃ X (X=Cl, Br, and I) boracites. <i>Physical Review B</i> , 2009 , 79,	3.3	3
41	CaFeO ₂ : a new type of layered structure with iron in a distorted square planar coordination. <i>Journal of the American Chemical Society</i> , 2009 , 131, 221-9	16.4	80
40	Raman Imaging Approach to the Study of Ferroelectric Domains and Raman Spectra of Multiferroic Boracites. <i>Acta Physica Polonica A</i> , 2009 , 116, 19-24	0.6	14
39	Hybrid exchange-correlation functional for accurate prediction of the electronic and structural properties of ferroelectric oxides. <i>Physical Review B</i> , 2008 , 77,	3.3	265
38	Modelling of carbon-based materials for hydrogen storage 2008 , 205-220		1
37	Phonons and magnetoelectric interactions in Ni ₃ V ₂ O ₈ . <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 434214	1.8	9
36	Theoretical investigation of hydrogen storage in metal-intercalated graphitic materials. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 285212	1.8	14
35	Structural and electronic properties of SrFeO ₂ from first principles. <i>Physical Review B</i> , 2008 , 78,	3.3	63
34	First-principles approach to lattice-mediated magnetoelectric effects. <i>Physical Review Letters</i> , 2008 , 101, 117201	7.4	79
33	Vibrational properties of TiH _n complexes adsorbed on carbon nanostructures. <i>Chemical Physics Letters</i> , 2007 , 444, 140-144	2.5	15
32	Hydrogen-related catalytic effects of Ti and other light transition metals on NaAlH ₄ surfaces. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 176007	1.8	8
31	Theoretical phase diagram of ultrathin films of incipient ferroelectrics. <i>Applied Physics Letters</i> , 2007 , 90, 242918	3.4	18
30	First-principles simulations on the nature of the melting line of sodium. <i>Physical Review Letters</i> , 2007 , 98, 055501	7.4	32
29	Effects of vacancies on the properties of disordered ferroelectrics: A first-principles study. <i>Physical Review B</i> , 2007 , 75,	3.3	19

28	Symmetry breaking at the nanoscale and diffuse transitions in ferroelectrics: A comparative study of $\text{PbSc}_{1-x}\text{Nb}_x\text{O}_3$ and $\text{PbZr}_{0.6}\text{Ti}_{0.4}\text{O}_3$. <i>Physical Review B</i> , 2006 , 73,	3-3	18
27	Amorphization induced by pressure: results for zeolites and general implications. <i>Physical Review Letters</i> , 2006 , 97, 225502	7-4	42
26	First-principles study of Ti-doped sodium alanate surfaces. <i>Applied Physics Letters</i> , 2005 , 86, 103109	3-4	58
25	Molecular and dissociative adsorption of multiple hydrogen molecules on transition metal decorated C_{60} . <i>Physical Review B</i> , 2005 , 72,	3-3	204
24	Unusual structural tuning of magnetism in cuprate perovskites. <i>Physical Review B</i> , 2005 , 71,	3-3	8
23	Atomistic simulations of the incipient ferroelectric KTaO_3 . <i>Physical Review B</i> , 2004 , 70,	3-3	47
22	Structure and hydrogen dynamics of pure and Ti-doped sodium alanate. <i>Physical Review B</i> , 2004 , 70,	3-3	138
21	Dynamics of Berry-phase polarization in time-dependent electric fields. <i>Physical Review B</i> , 2004 , 69,	3-3	73
20	Orbital and Spin Chains in ZnV_2O_4 . <i>Physical Review Letters</i> , 2004 , 93, 156407	7-4	128
19	THERMALLY DILUTED ISING SYSTEMS. <i>Fractals</i> , 2003 , 11, 53-65	3-2	10
18	Effects of atomic short-range order on the properties of perovskite alloys in their morphotropic phase boundary. <i>Physical Review Letters</i> , 2003 , 91, 045504	7-4	21
17	First-principles study of $(\text{BiScO}_3)_{1-x}(\text{PbTiO}_3)_x$ piezoelectric alloys. <i>Physical Review B</i> , 2003 , 67,	3-3	144
16	Quantitative analysis of the first-principles effective Hamiltonian approach to ferroelectric perovskites. <i>Physical Review B</i> , 2003 , 67,	3-3	41
15	Pressure amorphization through displacive disorder. <i>European Physical Journal E</i> , 2002 , 9, 239-43	1-5	4
14	Optical phonons associated with the low-temperature ferroelectric properties of perovskite solid solutions. <i>Physical Review B</i> , 2002 , 65,	3-3	22
13	First-principles study of the temperature-pressure phase diagram of BaTiO_3 . <i>Physical Review Letters</i> , 2002 , 89, 115503	7-4	94
12	First-principles approach to insulators in finite electric fields. <i>Physical Review Letters</i> , 2002 , 89, 117602	7-4	300
11	Flat branches and pressure amorphization. <i>Journal of Non-Crystalline Solids</i> , 2002 , 307-310, 602-612	3-9	16

10	Anomalous properties in ferroelectrics induced by atomic ordering. <i>Nature</i> , 2001 , 413, 54-7	50.4	76
9	Ab initio design of perovskite alloys with predetermined properties: the case of $\text{Pb}(\text{Sc}(0.5)\text{Nb}(0.5))\text{O}_3$. <i>Physical Review Letters</i> , 2001 , 87, 095503	7.4	43
8	Devonshire-Landau free energy of BaTiO_3 from first principles. <i>Physical Review B</i> , 2001 , 63,	3.3	43
7	Universality class of thermally diluted ising systems at criticality. <i>Physical Review E</i> , 2000 , 62, 191-6	2.4	13
6	Optimized local modes for lattice-dynamical applications. <i>Physical Review B</i> , 2000 , 61, 3127-3130	3.3	10
5	First-principles study of the structural instabilities in hexagonal barium titanate: Coupling between the soft optical and the acoustic Modes. <i>Ferroelectrics</i> , 2000 , 237, 25-32	0.6	2
4	Analysis of soft optical modes in hexagonal BaTiO_3 : transference of perovskite local distortions. <i>Journal of Physics Condensed Matter</i> , 2000 , 12, L387-L391	1.8	6
3	Self-averaging of random and thermally disordered diluted Ising systems. <i>Physical Review E</i> , 1999 , 60, 2394-7	2.4	16
2	Energetic Couplings in Ferroics. <i>Advanced Electronic Materials</i> , 2100639	6.4	0
1	Nanosession: Interplay Between Strain and Electronic Structure in Metal Oxides 377-387		