Ronald Cohen

List of Publications by Year
in descending order

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231	19,373	19636 61	11303 136
papers	citations	h-index	g-index

237	237	237	11722
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Origin of ferroelectricity in perovskite oxides. Nature, 1992, 358, 136-138.	13.7	2,629
2	Polarization rotation mechanism for ultrahigh electromechanical response in single-crystal piezoelectrics. Nature, 2000, 403, 281-283.	13.7	1,931
3	More accurate generalized gradient approximation for solids. Physical Review B, 2006, 73, .	1.1	1,785
4	Origin of morphotropic phase boundaries in ferroelectrics. Nature, 2008, 451, 545-548.	13.7	759
5	Lattice dynamics and origin of ferroelectricity inBaTiO3: Linearized-augmented-plane-wave total-energy calculations. Physical Review B, 1990, 42, 6416-6423.	1.1	567
6	Electronic structure studies of the differences in ferroelectric behavior of batio₃and PbTiO₃. Ferroelectrics, 1992, 136, 65-83.	0.3	367
7	First-principles elastic constants for the hcp transition metals Fe, Co, and Re at high pressure. Physical Review B, 1999, 60, 791-799.	1.1	355
8	Transformation of stishovite to a denser phase at lower-mantle pressures. Nature, 1995, 374, 243-245.	13.7	311
9	Magnetic Collapse in Transition Metal Oxides at High Pressure: Implications for the Earth. Science, 1997, 275, 654-657.	6.0	305
10	Pressure-Induced Anomalous Phase Transitions and Colossal Enhancement of Piezoelectricity inPbTiO3. Physical Review Letters, 2005, 95, 037601.	2.9	284
11	Theoretical determination of strong electron-phonon coupling inYBa2Cu3O7. Physical Review Letters, 1990, 64, 2575-2578.	2.9	279
12	Tight-binding total-energy method for transition and noble metals. Physical Review B, 1994, 50, 14694-14697.	1.1	258
13	Hard superconducting nitrides. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 3198-3201.	3.3	256
14	High-Pressure Elasticity of Iron and Anisotropy of Earth's Inner Core. Science, 1995, 267, 1972-1975.	6.0	254
15	Elasticity of iron at the temperature of the Earth's inner core. Nature, 2001, 413, 57-60.	13.7	240
16	First-Principles Study of Piezoelectricity inPbTiO3. Physical Review Letters, 1998, 80, 4321-4324.	2.9	226
17	Iron at high pressure: Linearized-augmented-plane-wave computations in the generalized-gradient approximation. Physical Review B, 1994, 50, 6442-6445.	1.1	225
18	Analysis of electronic structure and charge density of the high-temperature superconductor YBa2Cu3O7. Journal of Superconductivity and Novel Magnetism, 1988, 1, 111-141.	0.5	220

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19	Precise band structure and Fermi-surface calculation forYBa2Cu3O7: Importance of three-dimensional dispersion. Physical Review B, 1990, 42, 8764-8767.	1.1	194
20	Fermi Surfaces, Fermi Liquids, and High-Temperature Superconductors. Science, 1992, 255, 46-54.	6.0	191
21	Trends in elasticity and electronic structure of transition-metal nitrides and carbides from first principles. Physical Review B, 2005, 71, .	1.1	186
22	Lattice instabilities, isotope effect, and high-Tcsuperconductivity inLa2âˆ'xBaxCuO4. Physical Review Letters, 1991, 67, 228-231.	2.9	165
23	Thermal properties of iron at high pressures and temperatures. Physical Review B, 1996, 53, 8296-8309.	1.1	163
24	Accuracy of equation-of-state formulations. American Mineralogist, 2000, 85, 338-344.	0.9	160
25	Linearized augmented plane wave electronic structure calculations for MgO and CaO. Journal of Geophysical Research, 1988, 93, 8009-8022.	3.3	156
26	Calculated elastic and thermal properties of MGO at high pressures and temperatures. Journal of Geophysical Research, 1990, 95, 7055-7067.	3.3	154
27	First-Principles Phonon Calculations forLa2CuO4. Physical Review Letters, 1989, 62, 831-834.	2.9	153
28	Comparison of the electronic structures and energetics of ferroelectricLiNbO3andLiTaO3. Physical Review B, 1996, 53, 1193-1204.	1.1	146
29	Comparing the weighted density approximation with the LDA and GGA for ground-state properties of ferroelectric perovskites. Physical Review B, 2004, 70, .	1.1	139
30	Large calculated electron-phonon interactions inLa2âˆ'xMxCuO4. Physical Review B, 1993, 47, 1002-1015.	1.1	137
31	Composition and temperature of Earth's inner core. Journal of Geophysical Research, 1997, 102, 24729-24739.	3.3	129
32	Theory of ferroelectrics: a vision for the next decade and beyond. Journal of Physics and Chemistry of Solids, 2000, 61, 139-146.	1.9	129
33	Stability of orthorhombic MgSiO3 perovskite in the Earth's lower mantle. Nature, 1993, 364, 613-616.	13.7	127
34	High-pressure thermoelasticity of body-centered-cubic tantalum. Physical Review B, 2002, 65, .	1.1	122
35	Calculation of elasticity and high pressure instabilities in corundum and stishovite with the Potential Induced Breathing Model. Geophysical Research Letters, 1987, 14, 37-40.	1.5	120
36	Lattice dynamics of the potential-induced breathing model: Phonon dispersion in the alkaline-earth oxides. Physical Review B, 1987, 35, 5749-5760.	1.1	116

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37	Elasticity and equation of state of MgSiO₃ perovskite. Geophysical Research Letters, 1987, 14, 1053-1056.	1.5	115
38	High Sensitivity of Positrons to Oxygen Vacancies and to Copper-Oxygen Chain Disorder inYBa2Cu3O7â^'x. Physical Review Letters, 1988, 60, 2198-2201.	2.9	112
39	Experimental and Theoretical Evidence for Pressure-Induced Metallization in FeO with Rocksalt-Type Structure. Physical Review Letters, 2012, 108, 026403.	2.9	111
40	Giant Electrocaloric Effect Around<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:math>. Physical Review Letters, 2012, 109, 187604.	2.9	108
41	Iron-rich silicates in the Earth's D'' layer. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 9751-9753.	3.3	100
42	Effect of chemistry on the stability and elasticity of the perovskite and post-perovskite phases in the MgSiO3-FeSiO3-Al2O3system and implications for the lowermost mantle. Geophysical Research Letters, 2005, 32, .	1.5	100
43	Ionic contributions to lattice instabilities and phonon dispersion inLa2CuO4. Physical Review Letters, 1988, 60, 817-820.	2.9	99
44	Tight-binding computations of elastic anisotropy of Fe, Xe, and Si under compression. Physical Review B, 1997, 56, 8575-8589.	1.1	99
45	First-principles study of piezoelectricity in tetragonalPbTiO3andPbZr1/2Ti1/2O3. Physical Review B, 1999, 59, 12771-12776.	1.1	99
46	Mineralogy and petrology of chondrules and inclusions in the Mokoia CV3 chondrite. Geochimica Et Cosmochimica Acta, 1983, 47, 1739-1757.	1.6	98
47	Thermal equation of state of tantalum. Physical Review B, 2001, 63, .	1.1	87
48	Magnetism in dense hexagonal iron. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 33-36.	3.3	87
49	Silicate Perovskite. Annual Review of Earth and Planetary Sciences, 1992, 20, 553-600.	4.6	84
50	Surface effects in ferroelectrics: Periodic slab computations for BaTiO3. Ferroelectrics, 1997, 194, 323-342.	0.3	83
51	First-principles thermal equation of state and thermoelasticity of hcp Fe at high pressures. Physical Review B, 2010, 81, .	1.1	82
52	Relaxors go critical. Nature, 2006, 441, 941-942.	13.7	79
53	Raman spectroscopy and theoretical modeling of BeO at high pressure. Physical Review B, 1988, 37, 4727-4734.	1.1	72
54	Theoretical studies of charge relaxation effects on the statics and dynamics of oxides. Physics and Chemistry of Minerals, 1987, 14, 294-302.	0.3	71

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55	Structure, metal-insulator transitions, and magnetic properties of FeO at high pressures. American Mineralogist, 2003, 88, 257-261.	0.9	68
56	Lattice dynamics and thermodynamics of bcc iron under pressure: First-principles linear response study. Physical Review B, 2006, 73, .	1.1	68
57	Constraints on the crystalline structure of the inner core: Mechanical instability of BCC iron at high pressure. Geophysical Research Letters, 1995, 22, 125-128.	1.5	66
58	High pressure effects on thermal properties of MgO. Geophysical Research Letters, 1995, 22, 1533-1536.	1.5	66
59	Strong pressure-dependent electron-phonon coupling in FeSe. Physical Review B, 2014, 89, .	1.1	66
60	Origin of Negative Longitudinal Piezoelectric Effect. Physical Review Letters, 2017, 119, 207601.	2.9	63
61	Effects of Pressure on Diffusion and Vacancy Formation in MgO from Nonempirical Free-Energy Integrations. Physical Review Letters, 1997, 79, 3198-3201.	2.9	62
62	Possible polytypism in FeO at high pressures. American Mineralogist, 1998, 83, 451-457.	0.9	61
63	Carbon-boron clathrates as a new class of sp ³ -bonded framework materials. Science Advances, 2020, 6, eaay8361.	4.7	61
64	Periodic slab LAPW computations for ferroelectric BaTiO3. Journal of Physics and Chemistry of Solids, 1996, 57, 1393-1396.	1.9	60
65	Thermal Conductivity and Electrical Resistivity of Solid Iron at Earthâ€™s Core Conditions from First Principles. Physical Review Letters, 2018, 121, 096601.	2.9	60
66	Positron annihilation in high-Tcsuperconductors. Physical Review B, 1989, 39, 9667-9670.	1.1	58
67	Phase stability of wÃ¼stite at high pressure from first-principles linearized augmented plane-wave calculations. Physical Review B, 1993, 47, 7720-7731.	1.1	56
68	Melting and melt structure of MgO at high pressures. Physical Review B, 1994, 50, 12301-12311.	1.1	56
69	First-principles thermoelasticity of bcc iron under pressure. Physical Review B, 2006, 74, .	1.1	55
70	First-principles based atomistic modeling of phase stability in PMNâ€“xPT. Journal of Physics Condensed Matter, 2011, 23, 435902.	0.7	55
71	Electric-field-induced phase transition and electrocaloric effect in PMN-PT. Physical Review B, 2017, 96, .	1.1	54
72	Magnetism in iron as a function of pressure. Journal of Physics Condensed Matter, 2004, 16, S1109-S1119.	0.7	53

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73	Anomalous optical and electronic properties of dense sodium. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6525-6528.	3.3	53
74	Origin of diffuse scattering in relaxor ferroelectrics. Physical Review B, 2010, 81, .	1.1	53
75	Effects of electron correlations on transport properties of iron at Earthâ€™s core conditions. Nature, 2015, 517, 605-607.	13.7	53
76	Absence of lattice strain anomalies at the electronic topological transition in zinc at high pressure. Physical Review B, 2001, 63, .	1.1	52
77	Phase transitions and elasticity in zirconia. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1988, 150, 1-9.	0.9	50
78	Anharmonicity and the inverse isotope effect in the palladium-hydrogen system. Physical Review B, 1992, 45, 12405-12414.	1.1	50
79	The relationship between shear and compressional velocities at high pressures: Reconciliation of seismic tomography and mineral physics. Geophysical Research Letters, 1992, 19, 741-744.	1.5	50
80	Prediction of a new phase transition in Al2O3at high pressures. Geophysical Research Letters, 2005, 32, .	1.5	50
81	Reconciliation of Experiments and Theory on Transport Properties of Iron and the Geodynamo. Physical Review Letters, 2020, 125, 078501.	2.9	47
82	Ab initiolinear response and frozen phonons for the relaxorPbMg1âˆ•3Nb2âˆ•3O3. Physical Review B, 2005, 71, .	1.1	44
83	Quantum Monte Carlo computations of phase stability, equations of state, and elasticity of high-pressure silica. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9519-9524.	3.3	43
84	Atomistic Model Potential for PbTiO3and PMN by Fitting First Principles Results. Ferroelectrics, 2004, 301, 55-59.	0.3	42
85	Elastic isotropy of É›â€Fe under Earth's core conditions. Geophysical Research Letters, 2010, 37, .	1.5	42
86	High-pressure Raman scattering and x-ray diffraction of the relaxor ferroelectric0.96Pb(Zn1âˆ•3Nb2âˆ•3)O3â€“0.04PbTiO3. Physical Review B, 2005, 71, .	1.1	41
87	Ferrous iron in post-perovskite from first-principles calculations. Physics of the Earth and Planetary Interiors, 2008, 168, 147-152.	0.7	40
88	First-principles studies of electrical resistivity of iron under pressure. Journal of Physics Condensed Matter, 2011, 23, 075401.	0.7	40
89	Theoretical determination of the Raman spectra of MgSiO3perovskite and post-perovskite at high pressure. Geophysical Research Letters, 2006, 33, .	1.5	39
90	Measuring the melting curve of iron at super-Earth core conditions. Science, 2022, 375, 202-205.	6.0	39

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91	Fundamental High-Pressure Calibration from All-Electron Quantum MonteÂCarlo Calculations. Physical Review Letters, 2010, 104, 185702.	2.9	36
92	Origin of pyroelectricity in LiNbO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2011, 83, .	1.1	36
93	Raman measurements of phase transitions in dense solid hydrogen and deuterium to 325 GPa. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 4792-4797.	3.3	35
94	Thermodynamic solution properties of aluminous clinopyroxenes: Nonlinear least squares refinements. Geochimica Et Cosmochimica Acta, 1986, 50, 563-575.	1.6	34
95	First principles force field for metallic tantalum. Modelling and Simulation in Materials Science and Engineering, 2004, 12, S445-S459.	0.8	34
96	Applications of ionic models to the high-temperature superconductor La2CuO4. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1988, 150, 61-73.	0.9	33
97	Insulator-metal transition in solid hydrogen: Implication of electronic-structure calculations for recent experiments. Physical Review B, 1995, 52, R8597-R8600.	1.1	33
98	Comment on ÂOn the importance of the free energy for elasticity under pressureÂ. Journal of Physics Condensed Matter, 2004, 16, 8783-8786.	0.7	33
99	Response of Methylammonium Lead Iodide to External Stimuli and Caloric Effects from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 17274-17281.	1.5	33
100	Constraints on lower mantle composition from molecular dynamics simulations of MgSiO3 perovskite. Physics of the Earth and Planetary Interiors, 2002, 134, 239-252.	0.7	32
101	Pressure induced phase transitions in PbTiO3. Journal of Physics Condensed Matter, 2009, 21, 064225.	0.7	32
102	Electronic structure of calcium hexaboride within the weighted density approximation. Physical Review B, 2004, 69, .	1.1	31
103	Non-collinear magnetism in iron at high pressures. Physics of the Earth and Planetary Interiors, 2004, 143-144, 445-453.	0.7	31
104	Calculation of the electric field gradients at `tricluster'-like O atoms in the polymorphs of Al2SiO5 and in aluminosilicate molecules: models for tricluster O atoms in glasses. Journal of Non-Crystalline Solids, 2001, 286, 187-199.	1.5	29
105	Electronic stiffness of a superconducting niobium nitride single crystal under pressure. Physical Review B, 2005, 72, .	1.1	29
106	First-Principles Predictions of Elasticity and Phase Transitions in High Pressure SiO₂and Geophysical Implications. Geophysical Monograph Series, 0, , 425-431.	0.1	29
107	Origin of ferroelectricity in LiNbO3and LiTaO3. Ferroelectrics, 1997, 194, 83-95.	0.3	28
108	Thermal effects on lattice strain inÎµâ^'Feunder pressure. Physical Review B, 2006, 74, .	1.1	28

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109	Diffusion in MgO at high pressure: Implications for lower mantle rheology. Geophysical Research Letters, 1998, 25, 1095-1098.	1.5	27
110	Absence of Magnetism in Hcp Iron-Nickel at 11 K. Physical Review Letters, 2006, 97, 087202.	2.9	27
111	Post-perovskite phase in selected sesquioxides from density-functional calculations. Physical Review B, 2007, 76, .	1.1	27
112	Reply to â€œComment on â€˜More accurate generalized gradient approximation for solidsâ€™â€•. Physical Review B, 2008, 78, .	1.1	27
113	Raman spectroscopy and lattice dynamics of MgSiO₃-perovskite at high pressure. Geophysical Monograph Series, 0, , 35-44.	0.1	26
114	Pressure suppression of electron correlation in the collapsed tetragonal phase of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">CaFe</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mi mathvariant="normal">As</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>: A DFT-DMFT investigation. Physical Review B, 2014, 90, .	1.1	26
115	Structural diversity in lithium carbides. Physical Review B, 2015, 92, .	1.1	26
116	Weighted-density-approximation description of rare-earth trihydrides. Physical Review B, 2004, 69, .	1.1	25
117	Vacancy formation enthalpy at high pressures in tantalum. Journal of Physics Condensed Matter, 2003, 15, 855-861.	0.7	24
118	Brillouin scattering and molecular dynamics study of the elastic properties ofPb(Mg1â^•3Nb2â^•3)O3. Physical Review B, 2007, 75, .	1.1	24
119	Pressure dependence of the monoclinic phase in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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127	Electronic excitations and metallization of dense solid hydrogen. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13757-13762.	3.3	20
128	Graphene physics and insulator-metal transition in compressed hydrogen. Physical Review B, 2013, 88, .	1.1	19
129	Chemical accuracy from quantum Monte Carlo for the benzene dimer. Journal of Chemical Physics, 2015, 143, 104301.	1.2	19
130	Prediction of polar ordered oxynitride perovskites. Applied Physics Letters, 2007, 91, .	1.5	18
131	Molecular dynamics study of pbtio3using non-empirical potentials. Ferroelectrics, 1992, 136, 113-124.	0.3	17
132	Notes on the static dielectric response function in the density functional theory. Ferroelectrics, 1997, 194, 263-270.	0.3	17
133	Thermo-electromechanical response of a ferroelectric perovskite from molecular dynamics simulations. Applied Physics Letters, 2011, 99, .	1.5	17
134	Multiscale simulations of defect dipoleâ€“enhanced electromechanical coupling at dilute defect concentrations. Applied Physics Letters, 2017, 111, .	1.5	17
135	Quasiparticle scattering across the Fermi surface in La2-xMxCuO4. Physica B: Condensed Matter, 1990, 165-166, 1055-1056.	1.3	16
136	Origin of ferroelectricity in perovskites: The principal problems from a theoretical perspective. Ferroelectrics, 1993, 150, 1-12.	0.3	16
137	Pressure-volume-temperature equation of state of MgSiO3 perovskite from molecular dynamics and constraints on lower mantle composition. Journal of Geophysical Research, 2001, 106, 8615-8627.	3.3	16
138	Interpenetrating graphene networks: Three-dimensional node-line semimetals with massive negative linear compressibilities. Physical Review B, 2016, 94, .	1.1	16
139	Giant electrocaloric effect at the antiferroelectric-to-ferroelectric phase boundary in Pb(ZrxTi1â€“x)O3. Applied Physics Letters, 2019, 115, .	1.5	16
140	Linearized augmented plane wave total energy calculations for ferroelectric BaTiO₃. Ferroelectrics, 1990, 111, 57-61.	0.3	15
141	Origin of ferroelectricity in LiTaO3 and LiNbO3; LAPW total energy calculations. Ferroelectrics, 1995, 164, 45-55.	0.3	15
142	High-pressure Brillouin scattering of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Pb</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:msub><mml:mrow	1.1	15
	Physical Review B, 2009, 79, .		
143	Origin of stationary domain wall enhanced ferroelectric susceptibility. Physical Review B, 2017, 95, .	1.1	15
144	HighT_csuperconductors as ionic metals and the role of phonons in highT_csuperconductivity. Phase Transitions, 1990, 22, 167-183.	0.6	14

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145	Chapter 19. THEORY OF MINERALS AT HIGH PRESSURE. , 1998, , 639-672.		14
146	First-principles calculation of the formation energy in MgO-CaO solid solutions. Physical Review B, 2002, 65, .	1.1	14
147	Gregoryanzet al.Reply:. Physical Review Letters, 2003, 90, .	2.9	14
148	Pressure effects on relaxor ferroelectricity in disordered Pb(Sc1/2Nb1/2)O3. Journal of Applied Physics, 2010, 107, 074110.	1.1	14
149	Configurational thermodynamics of aluminous pyroxenes: A generalized pair approximation. Physics and Chemistry of Minerals, 1986, 13, 183-197.	0.3	13
150	Ferroelectricity origins. Nature, 1993, 362, 213-213.	13.7	13
151	Orbital ordering, ferroelasticity, and the large pressure-induced volume collapse in PbCrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2011, 83, .	1.1	13
152	Electronic structure and electron-phonon coupling in layered copper oxide superconductors. Physica B: Condensed Matter, 1991, 169, 45-50.	1.3	12
153	The melting curve and premelting of MgO. Geophysical Monograph Series, 1998, , 185-196.	0.1	12
154	Single-domain electromechanical constants for Pb(Zn1â•3Nb2â•3)O3â€“4.5%PbTiO3 from micro-Brillouin scattering. Applied Physics Letters, 2006, 88, 042908.	1.5	12
155	Effects of manganese addition on the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m Physical Review B, 2015, 91, .	1.1	12
156	Prediction of an Extended Ferroelectric Clathrate. Physical Review Letters, 2020, 125, 127601.	2.9	12
157	Effect of chemistry on the physical properties of perovskite and post-perovskite. Geophysical Monograph Series, 2007, , 115-128.	0.1	12
158	Statistical mechanics of coupled solid solutions in the dilute limit. Physics and Chemistry of Minerals, 1986, 13, 174-182.	0.3	11
159	Exciton energy and its pressure dependence in alkali halides. Physical Review B, 1994, 50, 70-74.	1.1	11
160	First principles studies of the born effective charges and electronic dielectric tensors for the relaxor PMN (PbMg1/3Nb2/3O3). Computational Materials Science, 2006, 37, 152-158.	1.4	11
161	Electronic Structure and Total Energy Calculations for Oxide Perovskites and Superconductors. Geophysical Monograph Series, 0, , 55-66.	0.1	11
162	Equations of state and stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">MgSiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>perovskite and post-perovskite phases from quantum Monte Carlo simulations. Physical Review B, 2014, 90, .	1.1	11

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163	Low-pressure phase diagram of crystalline benzene from quantum Monte Carlo. Journal of Chemical Physics, 2016, 145, .	1.2	11
164	Synthesis of a polar ordered oxynitride perovskite. Physical Review B, 2017, 95, .	1.1	11
165	Thermal conductivity of Fe-Si alloys and thermal stratification in Earthâ€™s core. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	11
166	Development of a Shell Model Potential for Molecular Dynamics for PbTiO3 by Fitting First Principles Results. AIP Conference Proceedings, 2002, , .	0.3	10
167	Ab initio Study of Elastic Properties of Pb(Ti,Zr)O3. AIP Conference Proceedings, 2002, , .	0.3	10
168	Stable charged antiparallel domain walls in hyperferroelectrics. Journal of Physics Condensed Matter, 2017, 29, 244003.	0.7	10
169	Hydrous SiO2 in subducted oceanic crust and H2O transport to the core-mantle boundary. Earth and Planetary Science Letters, 2022, 594, 117708.	1.8	10
170	Possiblity ofLiPdHxas a new ionic superconductor. Physical Review B, 1990, 41, 861-864.	1.1	9
171	Tight-binding based non-collinear spin model and magnetic correlations in iron. Journal of Computer-Aided Materials Design, 2001, 8, 107-115.	0.7	9
172	Effect of substrate temperature on structural and magnetic properties of c-axis oriented spinel ferrite Ni0.65Zn0.35Fe2O4 (NZFO) thin films. Journal of Alloys and Compounds, 2018, 766, 1074-1079.	2.8	9
173	First principles calculations for ferroelectrics â€” a vision. Ferroelectrics, 1990, 111, 1-7.	0.3	8
174	Prediction of a potential high-pressure structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">FeSiO</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	1.1	8
175	Ferroelectric polymers morph into action. Nature, 2018, 562, 48-49.	13.7	8
176	Valence and spin fluctuations in the Mn-doped ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2018, 98, .	1.1	8
177	Chapter 11. FIRST-PRINCIPLES THEORY OF CRYSTALLINE SiO2. , 1994, , 369-402.		7
178	Electrons, Phonons, and Electron-Phonon Interactions in High-Temperature Superconductors. Computers in Physics, 1994, 8, 34.	0.6	7
179	Physical properties of iron in the inner core. Geodynamic Series, 2003, , 137-161.	0.1	7
180	Undead layers breathe new life. Nature Materials, 2009, 8, 366-368.	13.3	7

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