David Price

List of Publications by Year
in descending order

188 papers	11,345 citations	20797 60 h-index	33869 99 g-index
193 all docs	193 docs citations	193 times ranked	6222 citing authors

#	Article	IF	Citations
1	Ab initiomolecular dynamics with variable cell shape: Application toMgSiO3. Physical Review Letters, 1993, 70, 3947-3950.	2.9	301
2	Phonon Density of States of Iron up to 153 Gigapascals. Science, 2001, 292, 914-916.	6.0	284
3	Iron under Earthâ€™s core conditions: Liquid-state thermodynamics and high-pressure melting curve fromab initiocalculations. Physical Review B, 2002, 65, .	1.1	277
4	The melting curve of iron at the pressures of the Earth's core from ab initio calculations. Nature, 1999, 401, 462-464.	13.7	270
5	The viscosity of liquid iron at the physical conditions of the Earth's core. Nature, 1998, 392, 805-807.	13.7	259
6	Composition and temperature of the Earthâ€™s core constrained by combining ab initio calculations and seismic data. Earth and Planetary Science Letters, 2002, 195, 91-98.	1.8	257
7	Thermodynamics of hexagonal-close-packed iron under Earthâ€™s core conditions. Physical Review B, 2001, 64, .	1.1	252
8	Possible thermal and chemical stabilization of body-centred-cubic iron in the Earth's core. Nature, 2003, 424, 536-539.	13.7	249
9	The elastic constants of MgSiO3 perovskite at pressures and temperatures of the Earth's mantle. Nature, 2001, 411, 934-937.	13.7	190
10	Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. Nature, 2005, 438, 1004-1007.	13.7	188
11	Thermal expansion and crystal structure of cementite, Fe3C, between 4 and 600â€…K determined by time-of-flight neutron powder diffraction. Journal of Applied Crystallography, 2004, 37, 82-90.	1.9	186
12	Role of the crystal-field theory in determining the structures of spinels. Journal of the American Chemical Society, 1982, 104, 92-95.	6.6	181
13	The influence of potassium on core and geodynamo evolution. Geophysical Journal International, 2004, 156, 363-376.	1.0	174
14	Ab initio study of MgSiO3 and CaSiO3 perovskites at lower-mantle pressures. Physics of the Earth and Planetary Interiors, 1995, 90, 101-112.	0.7	168
15	Crystal structure of tetrapropylammonium fluoride-containing precursor to fluoride silicalite. Journal of the American Chemical Society, 1982, 104, 5971-5977.	6.6	152
16	First-principles modelling of Earth and planetary materials at high pressures and temperatures. Reports on Progress in Physics, 2006, 69, 2365-2441.	8.1	152
17	Structural stability of silica at high pressures and temperatures. Physical Review B, 2005, 71, .	1.1	146
18	Computer modelling of solid-state inorganic materials. Nature, 1990, 347, 243-248.	13.7	145

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19	Ab initio lattice dynamics and structural stability of MgO. Journal of Chemical Physics, 2003, 118, 10174-10182.	1.2	144
20	The properties of iron under core conditions from first principles calculations. Physics of the Earth and Planetary Interiors, 2003, 140, 101-125.	0.7	138
21	The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO3. Earth and Planetary Science Letters, 2005, 230, 1-10.	1.8	137
22	Ab initio elasticity and thermal equation of state of MgSiO3 perovskite. Earth and Planetary Science Letters, 2001, 184, 555-560.	1.8	133
23	Gross thermodynamics of two-component core convection. Geophysical Journal International, 2004, 157, 1407-1414.	1.0	131
24	Interatomic potentials for CaCO3 polymorphs (calcite and aragonite), fitted to elastic and vibrational data. Physics and Chemistry of Minerals, 1992, 19, 80.	0.3	129
25	Can the Earth's dynamo run on heat alone?. Geophysical Journal International, 2003, 155, 609-622.	1.0	128
26	Impact induced melting and the development of large igneous provinces. Earth and Planetary Science Letters, 2002, 202, 551-561.	1.8	126
27	The lattice dynamics and thermodynamics of the Mg2SiO4 polymorphs. Physics and Chemistry of Minerals, 1987, 15, 181-190.	0.3	125
28	Computer simulations of the structural and physical properties of the olivine and spinel polymorphs of Mg2SiO4. Physics and Chemistry of Minerals, 1984, 10, 209-216.	0.3	114
29	Simulation of the pre-melting behaviour of MgSiO3 perovskite at high pressures and temperatures. Nature, 1991, 351, 735-737.	13.7	114
30	Thermal expansion and crystal structure of FeSi between 4 and 1173 K determined by time-of-flight neutron powder diffraction. Physics and Chemistry of Minerals, 2002, 29, 132-139.	0.3	113
31	Electron petrography of shock-produced veins in the Tenham chondrite. Contributions To Mineralogy and Petrology, 1979, 71, 211-218.	1.2	111
32	Ab Initio Studies of Silica-Based Clusters. Part I. Energies and Conformations of Simple Clusters. Journal of Physical Chemistry A, 1999, 103, 3252-3267.	1.1	111
33	Modelling the effect of water on the surface structure and stability of forsterite. Physics and Chemistry of Minerals, 2000, 27, 332-341.	0.3	110
34	Comparative study of quasiharmonic lattice dynamics, molecular dynamics and Debye model applied to MgSiO3 perovskite. Physics of the Earth and Planetary Interiors, 2000, 122, 277-288.	0.7	108
35	The effect of ferromagnetism on the equation of state of Fe 3 C studied by first-principles calculations. Earth and Planetary Science Letters, 2002, 203, 567-575.	1.8	108
36	Crystal structure, compressibility and possible phase transitions in oldvarepsilon-FeSi studied by first-principles pseudopotential calculations. Acta Crystallographica Section B: Structural Science, 1999, 55, 484-493.	1.8	107

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37	Ab initio chemical potentials of solid and liquid solutions and the chemistry of the Earthâ€™s core. Journal of Chemical Physics, 2002, 116, 7127-7136.	1.2	107
38	First principles calculations on crystalline and liquid iron at Earth's core conditions. Faraday Discussions, 1997, 106, 205-218.	1.6	106
39	Constraints on the composition of the Earth's core from ab initio calculations. Nature, 2000, 405, 172-175.	13.7	100
40	An infrared and Raman study of carbonate glasses: implications for the structure of carbonatite magmas. Geochimica Et Cosmochimica Acta, 1995, 59, 927-937.	1.6	99
41	Ab Initio Studies of Silica-Based Clusters. Part II. Structures and Energies of Complex Clusters. Journal of Physical Chemistry A, 1999, 103, 3268-3284.	1.1	97
42	High-pressure (Mg, Fe)2SiO4 phases in the Tenham chondritic meteorite. Nature, 1979, 280, 217-218.	13.7	96
43	Synthesis of 1,4-dinitrocubane. Journal of Organic Chemistry, 1984, 49, 185-186.	1.7	93
44	Electronic spin transitions in iron-bearing MgSiO3 perovskite. Earth and Planetary Science Letters, 2007, 253, 282-290.	1.8	93
45	Molecular dynamics simulations of CaCO3 melts to mantle pressures and temperatures: implications for carbonatite magmas. Earth and Planetary Science Letters, 1995, 131, 225-238.	1.8	89
46	Ab initio free energy calculations on the polymorphs of iron at core conditions. Physics of the Earth and Planetary Interiors, 2000, 117, 123-137.	0.7	89
47	Complementary approaches to the ab initio calculation of melting properties. Journal of Chemical Physics, 2002, 116, 6170-6177.	1.2	88
48	Molecular dynamics simulations of vitreous silica structures. Journal of Non-Crystalline Solids, 2004, 345-346, 224-229.	1.5	87
49	Elasticity of CaSiO3 perovskite at high pressure and high temperature. Physics of the Earth and Planetary Interiors, 2006, 155, 249-259.	0.7	84
50	Temperature and composition of the Earth's core. Contemporary Physics, 2007, 48, 63-80.	0.8	84
51	The lattice dynamics of forsterite. Mineralogical Magazine, 1987, 51, 157-170.	0.6	83
52	Feî—¸Mg interdiffusion in olivine up to 9 GPa at T = 600â€“900Â°C; experimental data and comparison with defect calculations. Physics of the Earth and Planetary Interiors, 1995, 89, 199-218.	0.7	81
53	Phase changes and thermodynamic properties of CaTiO3. Spectroscopic data, vibrational modelling and some insights on the properties of MgSiO3 perovskite. Physics and Chemistry of Minerals, 1993, 20, 159-170.	0.3	80
54	The application of the ANNNI model to polytypic behaviour. Acta Crystallographica Section B: Structural Science, 1984, 40, 448-454.	1.8	77

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55	Thermal expansion and atomic displacement parameters of cubic KMgF3perovskite determined by high-resolution neutron powder diffraction. Journal of Applied Crystallography, 2002, 35, 291-295.	1.9	77
56	Systematic enumeration of zeolite frameworks. Zeolites, 1989, 9, 23-32.	0.9	74
57	Factors influencing solid-state structureâ€"an analysis using pseudopotential radii structural maps. Physical Review B, 1981, 24, 2903-2912.	1.1	69
58	Silica condensation reaction: an ab initio study. Chemical Communications, 1998, , 1387-1388.	2.2	68
59	The melting of MgO â€" computer calculations via molecular dynamics. Physics and Chemistry of Minerals, 1996, 23, 42-49.	0.3	64
60	The composition and geotherm of the lower mantle: constraints from the elasticity of silicate perovskite. Physics of the Earth and Planetary Interiors, 2000, 118, 103-109.	0.7	61
61	Neutron diffraction at simultaneous high temperatures and pressures, with measurement of temperature by neutron radiography. Mineralogical Magazine, 2001, 65, 737-748.	0.6	60
62	Melting curve of materials: theory versus experiments. Journal of Physics Condensed Matter, 2004, 16, S973-S982.	0.7	59
63	Elastic anisotropy of FeSiO3end-members of the perovskite and post-perovskite phases. Geophysical Research Letters, 2006, 33, n/a-n/a.	1.5	59
64	First principles calculations on the diffusivity and viscosity of liquid Feâ€"S at experimentally accessible conditions. Physics of the Earth and Planetary Interiors, 2000, 120, 145-152.	0.7	58
65	Electronic structure of the antiferromagneticB1-structured FeO. Physical Review B, 2004, 70, .	1.1	57
66	CaSiO3perovskite at lower mantle pressures. Geophysical Research Letters, 2005, 32, .	1.5	57
67	A spinel to Î²-phase transformation mechanism in (Mg,Fe)2SiO4. Nature, 1982, 296, 729-731.	13.7	53
68	Oxygen in the Earth's core: a first-principles study. Physics of the Earth and Planetary Interiors, 1999, 110, 191-210.	0.7	51
69	Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO3post-perovskite. Geophysical Research Letters, 2006, 33, .	1.5	50
70	High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores. Earth and Planetary Science Letters, 2008, 272, 481-487.	1.8	50
71	Molecular Dynamics Simulation of Methanolic and Ethanolic Silica-Based Solâ^'Gel Solutions at Ambient Temperature and Pressure. Journal of Physical Chemistry A, 2002, 106, 130-148.	1.1	49
72	Exsolution microstructures in titanomagnetites and their magnetic significance. Physics of the Earth and Planetary Interiors, 1980, 23, 2-12.	0.7	48

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73	Computer simulation of the MgSiO3 polymorphs. Physics and Chemistry of Minerals, 1992, 18, 365.	0.3	48
74	The GrÃ¼neisen parameter â€" computer calculations via lattice dynamics. Physics of the Earth and Planetary Interiors, 1994, 82, 261-270.	0.7	47
75	The structure of iron under the conditions of the Earth's inner core. Geophysical Research Letters, 1999, 26, 1231-1234.	1.5	47
76	Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. Geophysical Research Letters, 2005, 32, .	1.5	47
77	Phase stability of CaSiO3 perovskite at high pressure and temperature: Insights from ab initio molecular dynamics. Physics of the Earth and Planetary Interiors, 2006, 155, 260-268.	0.7	46
78	Absolute ionic diffusion in MgOâ€"computer calculations via lattice dynamics. Physics of the Earth and Planetary Interiors, 1995, 88, 193-210.	0.7	44
79	Computer modelling of B2O3. I. New interatomic potentials, crystalline phases and predicted polymorphs. Journal of Physics Condensed Matter, 1995, 7, 8659-8692.	0.7	43
80	Proton-containing defects at forsterite {010} tilt grain boundaries and stepped surfaces. American Mineralogist, 2000, 85, 1143-1154.	0.9	43
81	Elasticity of (Mg, Fe)(Si, Al)O3-perovskite at high pressure. Earth and Planetary Science Letters, 2005, 240, 529-536.	1.8	42
82	Computer simulation of defects and diffusion in perovskites. Journal of Geophysical Research, 1993, 98, 22245-22253.	3.3	41
83	The nature and significance of stacking faults in wadsleyite, natural Î²-(Mg, Fe)2SiO4 from the Peace River meteorite. Physics of the Earth and Planetary Interiors, 1983, 33, 137-147.	0.7	40
84	Primary slip system of Îµ-iron and anisotropy of the Earth's inner core. Physics of the Earth and Planetary Interiors, 1999, 110, 147-156.	0.7	40
85	The optical constants of ordinary glass from 0.29 to 4000 cm-1. Journal Physics D: Applied Physics, 1975, 8, 1353-1358.	1.3	39
86	Relative stability of zeolite frameworks from calculated energetics of known and theoretical structures. Zeolites, 1989, 9, 321-328.	0.9	39
87	A high-pressure study of â^Š-FeSi, between 0 and 8.5 GPa, by time-of-flight neutron powder diffraction. Journal of Applied Crystallography, 1996, 29, 215-218.	1.9	39
88	EVOLUTION AND PALEOGEOGRAPHIC DISTRIBUTION OF THE LEPIDOCYCLINIDS. Journal of Foraminiferal Research, 2010, 40, 79-108.	0.1	39
89	Ab initiothermodynamics and phase diagram of solid magnesium: A comparison of the LDA and GGA. Journal of Chemical Physics, 2006, 125, 194507.	1.2	38
90	The factors influencing cation site-preferences in spinels a new mendelyevian approach. Physics and Chemistry of Minerals, 1982, 8, 69-76.	0.3	37

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91	High-temperature creep of the perovskites CaTiO3 and NaNbO3. Physics of the Earth and Planetary Interiors, 1992, 74, 9-22.	0.7	37
92	Deriving empirical potentials for molecular ionic materials. Mineralogical Magazine, 1995, 59, 617-622.	0.6	37
93	Ab initio theory of planetary materials. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	37
94	High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al2O3. Geophysical Research Letters, 2005, 32, .	1.5	37
95	Thermal expansion of mantle minerals at high pressuresâ€"A theoretical study. Geophysical Research Letters, 1990, 17, 689-692.	1.5	36
96	Computer modelling of B2O3. II. Molecular dynamics simulations of vitreous structures. Journal of Physics Condensed Matter, 1995, 7, 8693-8722.	0.7	36
97	Electronic Structure Study of the High-pressure Vibrational Spectrum of FeS2Pyrite. Journal of Physical Chemistry B, 2005, 109, 22067-22073.	1.2	36
98	Ab initiototal-energy pseudopotential calculations for polymorphicB2O3crystals. Physical Review B, 1995, 51, 1447-1455.	1.1	35
99	Molecular Dynamics Simulation of Liquid H2O, MeOH, EtOH, Si(OMe)4, and Si(OEt)4, as a Function of Temperature and Pressure. Journal of Physical Chemistry A, 2001, 105, 1909-1925.	1.1	35
100	Computer modelling of a pressure induced phase change in clinoenstatite pyroxenes. Physics and Chemistry of Minerals, 1997, 25, 55-62.	0.3	34
101	Thermodynamics from first principles: temperature and composition of the Earthâ€™s core. Mineralogical Magazine, 2003, 67, 113-123.	0.6	34
102	Elasticity of Mg2SiO4 ringwoodite at mantle conditions. Physics of the Earth and Planetary Interiors, 2006, 157, 181-187.	0.7	34
103	The stability of bcc-Fe at high pressures and temperatures with respect to tetragonal strain. Physics of the Earth and Planetary Interiors, 2008, 170, 52-59.	0.7	34
104	Polytypism and the factors determining the stability of spinelloid structures. Physics and Chemistry of Minerals, 1983, 10, 77-83.	0.3	33
105	Crystal structure of tetrapropylammonium fluoride-silicalite. Nature, 1981, 292, 818-819.	13.7	32
106	First-principles simulation of high-pressure polymorphs in MgAl2O4. Physics and Chemistry of Minerals, 2008, 35, 381-386.	0.3	32
107	The ab initio simulation of the Earth's core. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2002, 360, 1227-1244.	1.6	31
108	Ab initio calculations on the free energy and high Pâ€“T elasticity of face-centred-cubic iron. Earth and Planetary Science Letters, 2008, 268, 444-449.	1.8	31

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109	The melting of MgO studied by molecular dynamics simulation. Modelling and Simulation in Materials Science and Engineering, 1994, 2, 1101-1110.	0.8	30
110	Comparison between the lattice dynamics and molecular dynamics methods: Calculation results for MgSiO3perovskite. Geophysical Research Letters, 1994, 21, 1659-1662.	1.5	30
111	The phylogenetic and palaeogeographic evolution of the miogypsinid larger benthic foraminifera. Journal of the Geological Society, 2013, 170, 185-208.	0.9	30
112	The properties and behaviour of mantle minerals: a computer-simulation approach. Philosophical Transactions of the Royal Society A, 1989, 328, 391-407.	1.3	29
113	Infrared spectroscopy of the polymorphic series (enstatite, ilmenite, and perovskite) of MgSiO₃, MgGeO₃, and MnGeO₃. Journal of Geophysical Research, 1989, 94, 15687-15701.	3.3	29
114	Theoretical investigation of metastable Al2SiO5polymorphs. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 548-557.	0.3	29
115	A computer simulation of the structure and elastic properties of MgSiO3 perovskite. Mineralogical Magazine, 1986, 50, 693-707.	0.6	28
116	Dislocations in CaTiO3 perovskite deformed at high-temperature: a transmission electron microscopy study. Physics and Chemistry of Minerals, 1996, 23, 337.	0.3	28
117	The melting curve of iron from quantum mechanics calculations. Journal of Physics and Chemistry of Solids, 2004, 65, 1573-1580.	1.9	28
118	Structural and magnetic phase transitions in simple oxides using hybrid functionals. Molecular Simulation, 2005, 31, 367-377.	0.9	28
119	Computer simulation of the infrared and Raman activity of pyrope garnet, and assignment of calculated modes to specific atomic motions. American Mineralogist, 1998, 83, 841-847.	0.9	27
120	The energetics of polytypic structures: a computer simulation of magnesium silicate spinelloids. Acta Crystallographica Section B: Structural Science, 1985, 41, 231-239.	1.8	26
121	Laboratory impact experiments versus natural impact events. , 2002, , .		26
122	Dopant control over the crystal morphology of ceramic materials. Surface Science, 2007, 601, 4793-4800.	0.8	26
123	Electrical conductivity of the lower mantle: a molecular dynamics simulation of MgSiO3 perovskite. Physics of the Earth and Planetary Interiors, 1989, 58, 192-204.	0.7	25
124	Ab initio molecular dynamics simulations for thermal equation of state of B2-type NaCl. Journal of Applied Physics, 2008, 103, 023510.	1.1	24
125	Diffusion in the titanomagnetite solid solution series. Mineralogical Magazine, 1981, 44, 195-200.	0.6	23
126	Elastic, thermal and structural properties of platinum. Journal of Physics and Chemistry of Solids, 2011, 72, 169-175.	1.9	23

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127	Site preference of vanadium doped into ZrSiO4 and ZrGeO4 and of terbium doped into ZrGeO4. Journal of the Chemical Society Dalton Transactions, 1992, , 1579.	1.1	22
128	Ab initiothermodynamics of MgSiO3 perovskite at high pressures and temperatures. Journal of Chemical Physics, 2005, 122, 124501.	1.2	22
129	Submillimeter-Wave Dielectric Measurements on Absorbing Materials. IEEE Transactions on Instrumentation and Measurement, 1974, 23, 483-488.	2.4	21
130	Industrial Applications of Simulation Studies in Solid State Chemistry. Molecular Simulation, 1989, 3, 49-69.	0.9	21
131	A simple, systematic method for the generation periodic, 2-dimensional, 3-connected nets for the description of zeolite frameworks. Zeolites, 1992, 12, 320-327.	0.9	21
132	Compressibility of FeSi between 0 and 9 GPa, determined by high pressure time-of-flight neutron powder diffraction. Journal of Physics Condensed Matter, 1995, 7, L475-L479.	0.7	21
133	Atomistic modeling of silica based sol-gel processes. Journal of Sol-Gel Science and Technology, 1997, 8, 55-58.	1.1	21
134	An ab initio study of the relative stabilities and equations of state of FeS polymorphs. Mineralogical Magazine, 2001, 65, 181-191.	0.6	21
135	Molecular dynamics simulation of polymorphic and polyamorphic transitions in tetrahedral network glasses: BeF2 and GeO2. Journal of Non-Crystalline Solids, 2007, 353, 1892-1898.	1.5	21
136	Molecular dynamics simulation of temperature-induced structural changes in cristobalite, coesite and amorphous silica. Journal of Non-Crystalline Solids, 2008, 354, 181-187.	1.5	21
137	Microstructures in titanomagnetites as guides to cooling rates of a Swedish intrusion. Geological Magazine, 1979, 116, 313-318.	0.9	20
138	A Transferable Interatomic Potential for Calcium Carbonate. Molecular Simulation, 1992, 9, 175-177.	0.9	20
139	Phase transitions of BaCO₃ at high pressures. Mineralogical Magazine, 2008, 72, 659-665.	0.6	20
140	A computer simulation study of the effect of pressure on Mg diffusion in forsterite. Physics of the Earth and Planetary Interiors, 2009, 172, 13-19.	0.7	20
141	Dispersive Fourier transform measurements on opaque solids from 5 to 350 cmâ˜'1. Infrared Physics, 1976, 16, 311-315.	0.5	19
142	POWDER NEUTRON-DIFFRACTION STUDIES OF CLINOPYROXENES. I. THE CRYSTAL STRUCTURE AND THERMOELASTIC PROPERTIES OF JADEITE BETWEEN 1.5 AND 270 K. Canadian Mineralogist, 2008, 46, 1593-1622.	0.3	18
143	The structural relation between svetlozarite and dachiardite. Mineralogical Magazine, 1982, 45, 157-161.	0.6	17
144	Thermodynamic and anharmonic properties of forsterite, Î±â€Mg₂SiO₄: Computer modelling versus highâ€pressure and highâ€temperature measurements. Journal of Geophysical Research, 1992, 97, 19791-19801.	3.3	17

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145	The influence of thermal vibrations on the average structure of cubic perovskite: a combined molecular dynamics and neutron diffraction study. Journal of Physics Condensed Matter, 1997, 9, L647-L655.	0.7	17
146	Thermodynamic Stability of Fe/O Solid Solution at Inner-Core Conditions. Geophysical Research Letters, 2000, 27, 2417-2420.	1.5	17
147	Crystal morphology and surface structures of orthorhombic MgSiO3 perovskite. Physics and Chemistry of Minerals, 2005, 31, 671-682.	0.3	17
148	The energetics of polytypic structures: further applications of the ANNNI model. Acta Crystallographica Section B: Structural Science, 1985, 41, 310-319.	1.8	16
149	Structures and physical properties of â^Š-FeSi-type and CsCl-type RuSi studied by first-principles pseudopotential calculations. Acta Crystallographica Section B: Structural Science, 2000, 56, 369-376.	1.8	16
150	Computational mineral physics and the physical properties of perovskite. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2002, 360, 2507-2520.	1.6	16
151	Thermoelastic properties of magnesiowÃ¼stite, (Mg_{1â^'x}Fe_x)O: determination of the Andersonâ€“GrÃ¼neisen parameter by time-of-flight neutron powder diffraction at simultaneous high pressures and temperatures. Journal of Applied Crystallography, 2008, 41, 886-896.	1.9	15
152	Ab initio molecular dynamics study of elasticity of akimotoite MgSiO3 at mantle conditions. Physics of the Earth and Planetary Interiors, 2009, 173, 115-120.	0.7	14
153	The effect of cation-ordering on the elastic properties of majorite: An ab initio study. Earth and Planetary Science Letters, 2007, 256, 28-35.	1.8	13
154	Ab initio molecular dynamic simulation on the elasticity of Mg3Al2Si3O12 pyrope. Journal of Earth Science (Wuhan, China), 2011, 22, 169-175.	1.1	13
155	A model for polysomatism. Mineralogical Magazine, 1986, 50, 149-156.	0.6	13
156	The nature and significance of exsolved phases in some chrome spinels from the Rhum layered intrusion. Mineralogical Magazine, 1979, 43, 519-526.	0.6	12
157	Dislocation melting of metals. Physics of the Earth and Planetary Interiors, 1992, 69, 153-162.	0.7	12
158	A mechanism for pyroxene-pyroxenoid and pyroxenoid-pyroxenoid transformations. Physics and Chemistry of Minerals, 1984, 10, 236-243.	0.3	11
159	The effect of many-body forces on the elastic properties of simple oxides and olivine. Physics and Chemistry of Minerals, 1988, 16, 42.	0.3	11
160	A computer simulation approach to the high pressure thermoelasticity of MgSiO3 perovskite. Physics of the Earth and Planetary Interiors, 1996, 98, 55-63.	0.7	11
161	The Computer Simulation of the Lattice Dynamics of Silicates. , 1988, , 591-618.		11
162	Computer simulations of iron in magnesium silicate perovskite. Geophysical Research Letters, 1989, 16, 1399-1402.	1.5	10

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163	A microscopic model for a very stable incommensurate modulated mineral: mullite. Journal of Physics Condensed Matter, 1993, 5, 3417-3430.	0.7	10
164	The factors influencing solid state structure â€" A modern Mendeleyevian answer. Solid State Communications, 1981, 40, 923-926.	0.9	9
165	A study of the structures and energetics of magnesium silicates. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1985, 131, 290-299.	0.9	9
166	Structural & physical properties of the binary transition metal- containing perovskite La2CoMnO6. Synthetic Metals, 2001, 121, 1467-1468.	2.1	9
167	High-temperature structural phase transitions in neighborite: a high-resolution neutron powder diffraction investigation. Physics and Chemistry of Minerals, 2015, 42, 45-52.	0.3	9
168	Periodic ab initio Hartree-Fock study of trigonal and orthorhombic phases of boric oxides. Physics and Chemistry of Minerals, 1997, 24, 423-431.	0.3	8
169	Ab initio study of the phase separation of argon in molten iron at high pressures. Geophysical Research Letters, 2006, 33, .	1.5	8
170	Structural phase transitions in IrO2at high pressures. Journal of Physics Condensed Matter, 2008, 20, 045202.	0.7	8
171	Oxidation phenomena in pleonaste bearing titanomagnetites. Contributions To Mineralogy and Petrology, 1979, 69, 355-359.	1.2	7
172	A new approach to simulating disorder in crystals. Physics and Chemistry of Minerals, 1990, 17, 238.	0.3	7
173	Molecular dynamics: some recent developments in classical and quantum mechanical simulation of minerals. Mineralogical Magazine, 1995, 59, 597-605.	0.6	7
174	An ab initio study of the relative stabilities and equations of state of Fe3S polymorphs. Mineralogical Magazine, 2004, 68, 813-817.	0.6	6
175	Crystal morphology and surface structures of orthorhombic MgSiO3 in the presence of divalent impurity ions. Physics and Chemistry of Minerals, 2005, 32, 379-387.	0.3	6
176	Defects and diffusion in MgSiO₃perovskite: a computer simulation. Geophysical Monograph Series, 0, , 45-53.	0.1	6
177	Exsolution in titanomagnetites as an indicator of cooling rates. Mineralogical Magazine, 1982, 46, 19-25.	0.6	5
178	Gravity glide and plate tectonics. Geological Society Special Publication, 1988, 37, 5-21.	0.8	5
179	The geographic, environmental and phylogenetic evolution of the Alveolinoidea from the Cretaceous to the present day. UCL Open Environment, 0, 2, .	0.0	5
180	Earth sciences: Perovskites and plate tectonics. Nature, 1986, 319, 175-175.	13.7	4

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