David Price

List of Publications by Citations

185 papers	9,781 citations	58 h-index	91 g-index
193 ext. papers	10,374 ext. citations	6.7 avg, IF	5.81 L-index

#	Paper	IF	Citations
185	Phonon density of states of iron up to 153 gigapascals. *Science*, **2001**, 292, 914-6	33.3	264
184	The melting curve of iron at the pressures of the Earth's core from ab initio calculations. *Nature*, **1999**, 401, 462-464	50.4	248
183	Ab initio molecular dynamics with variable cell shape: Application to MgSiO3. *Physical Review Letters*, **1993**, 70, 3947-3950	7.4	247
182	Iron under Earth's core conditions: Liquid-state thermodynamics and high-pressure melting curve from ab initio calculations. *Physical Review B*, **2002**, 65,	3.3	242
181	The viscosity of liquid iron at the physical conditions of the Earth's core. *Nature*, **1998**, 392, 805-807	50.4	232
180	Thermodynamics of hexagonal-close-packed iron under Earth's core conditions. *Physical Review B*, **2001**, 64,	3.3	230
179	Composition and temperature of the Earth's core constrained by combining ab initio calculations and seismic data. *Earth and Planetary Science Letters*, **2002**, 195, 91-98	5.3	221
178	Possible thermal and chemical stabilization of body-centred-cubic iron in the Earth's core. *Nature*, **2003**, 424, 536-9	50.4	219
177	Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. *Nature*, **2005**, 438, 1004-7	50.4	175
176	The elastic constants of MgSiO3 perovskite at pressures and temperatures of the Earth's mantle. *Nature*, **2001**, 411, 934-7	50.4	172
175	Thermal expansion and crystal structure of cementite, Fe3C, between 4 and 600 K determined by time-of-flight neutron powder diffraction. *Journal of Applied Crystallography*, **2004**, 37, 82-90	3.8	153
174	The influence of potassium on core and geodynamo evolution. *Geophysical Journal International*, **2004**, 156, 363-376	2.6	152
173	Ab initio study of MgSiO3 and CaSiO3 perovskites at lower-mantle pressures. *Physics of the Earth and Planetary Interiors*, **1995**, 90, 101-112	2.3	149
172	Role of the crystal-field theory in determining the structures of spinels. *Journal of the American Chemical Society*, **1982**, 104, 92-95	16.4	138
171	Crystal structure of tetrapropylammonium fluoride-containing precursor to fluoride silicalite. *Journal of the American Chemical Society*, **1982**, 104, 5971-5977	16.4	136
170	First-principles modelling of Earth and planetary materials at high pressures and temperatures. *Reports on Progress in Physics*, **2006**, 69, 2365-2441	14.4	133
169	Ab initio lattice dynamics and structural stability of MgO. *Journal of Chemical Physics*, **2003**, 118, 10174-10182	3.3	130

168	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	5.3	129
167	Computer modelling of solid-state inorganic materials. *Nature*, **1990**, 347, 243-248	50.4	127
166	The properties of iron under core conditions from first principles calculations. *Physics of the Earth and Planetary Interiors*, **2003**, 140, 101-125	2.3	126
165	Ab initio elasticity and thermal equation of state of MgSiO3 perovskite. *Earth and Planetary Science Letters*, **2001**, 184, 555-560	5.3	125
164	Structural stability of silica at high pressures and temperatures. *Physical Review B*, **2005**, 71,	3.3	121
163	Gross thermodynamics of two-component core convection. *Geophysical Journal International*, **2004**, 157, 1407-1414	2.6	116
162	Can the Earth's dynamo run on heat alone?. *Geophysical Journal International*, **2003**, 155, 609-622	2.6	108
161	Ab Initio Studies of Silica-Based Clusters. Part I. Energies and Conformations of Simple Clusters. *Journal of Physical Chemistry A*, **1999**, 103, 3252-3267	2.8	103
160	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	5.3	102
159	Impact induced melting and the development of large igneous provinces. *Earth and Planetary Science Letters*, **2002**, 202, 551-561	5.3	100
158	The lattice dynamics and thermodynamics of the Mg2SiO4 polymorphs. *Physics and Chemistry of Minerals*, **1987**, 15, 181-190	1.6	100
157	Simulation of the pre-melting behaviour of MgSiO3 perovskite at high pressures and temperatures. *Nature*, **1991**, 351, 735-737	50.4	99
156	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	2.3	97
155	Interatomic potentials for CaCO3 polymorphs (calcite and aragonite), fitted to elastic and vibrational data. *Physics and Chemistry of Minerals*, **1992**, 19, 80	1.6	96
154	First principles calculations on crystalline and liquid iron at Earth's core conditions. *Faraday Discussions*, **1997**, 106, 205-218	3.6	94
153	Modelling the effect of water on the surface structure and stability of forsterite. *Physics and Chemistry of Minerals*, **2000**, 27, 332-341	1.6	93
152	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	1.6	93
151	Ab initio chemical potentials of solid and liquid solutions and the chemistry of the Earth□ core. *Journal of Chemical Physics*, **2002**, 116, 7127-7136	3.9	92

150	Ab Initio Studies of Silica-Based Clusters. Part II. Structures and Energies of Complex Clusters. *Journal of Physical Chemistry A*, **1999**, 103, 3268-3284	2.8	92
149	Electron petrography of shock-produced veins in the Tenham chondrite. *Contributions To Mineralogy and Petrology*, **1979**, 71, 211-218	3.5	91
148	Crystal structure, compressibility and possible phase transitions in boldvarepsilon-FeSi studied by first-principles pseudopotential calculations. *Acta Crystallographica Section B: Structural Science*, **1999**, 55, 484-493		90
147	Electronic spin transitions in iron-bearing MgSiO3 perovskite. *Earth and Planetary Science Letters*, **2007**, 253, 282-290	5.3	89
146	High-pressure (Mg, Fe)2SiO4 phases in the Tenham chondritic meteorite. *Nature*, **1979**, 280, 217-218	50.4	89
145	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	1.6	88
144	Constraints on the composition of the Earth's core from ab initio calculations. *Nature*, **2000**, 405, 172-5	50.4	88
143	An infrared and Raman study of carbonate glasses: implications for the structure of carbonatite magmas. *Geochimica Et Cosmochimica Acta*, **1995**, 59, 927-937	5.5	83
142	Molecular dynamics simulations of CaCO3 melts to mantle pressures and temperatures: implications for carbonatite magmas. *Earth and Planetary Science Letters*, **1995**, 131, 225-238	5.3	80
141	Ab initio free energy calculations on the polymorphs of iron at core conditions. *Physics of the Earth and Planetary Interiors*, **2000**, 117, 123-137	2.3	79
140	Synthesis of 1,4-dinitrocubane. *Journal of Organic Chemistry*, **1984**, 49, 185-186	4.2	79
139	Complementary approaches to the ab initio calculation of melting properties. *Journal of Chemical Physics*, **2002**, 116, 6170-6177	3.9	77
138	The lattice dynamics of forsterite. *Mineralogical Magazine*, **1987**, 51, 157-170	1.7	74
137	Elasticity of CaSiO3 perovskite at high pressure and high temperature. *Physics of the Earth and Planetary Interiors*, **2006**, 155, 249-259	2.3	72
136	Molecular dynamics simulations of vitreous silica structures. *Journal of Non-Crystalline Solids*, **2004**, 345-346, 224-229	3.9	71
135	Temperature and composition of the Earth's core. *Contemporary Physics*, **2007**, 48, 63-80	3.3	67
134	The application of the ANNNI model to polytypic behaviour. *Acta Crystallographica Section B: Structural Science*, **1984**, 40, 448-454		66
133	Fe?Mg interdiffusion in olivine up to 9 GPa at T = 600?900°C; experimental data and comparison with defect calculations. *Physics of the Earth and Planetary Interiors*, **1995**, 89, 199-218	2.3	65

132	Systematic enumeration of zeolite frameworks. *Zeolites*, **1989**, 9, 23-32		64
131	Silica condensation reaction: an ab initio study. *Chemical Communications*, **1998**, 1387-1388	5.8	63
130	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	1.6	62
129	Factors influencing solid-state structure□n analysis using pseudopotential radii structural maps. *Physical Review B*, **1981**, 24, 2903-2912	3.3	62
128	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	2.3	58
127	The melting of MgO □omputer calculations via molecular dynamics. *Physics and Chemistry of Minerals*, **1996**, 23, 42-49	1.6	58
126	Melting curve of materials: theory versus experiments. *Journal of Physics Condensed Matter*, **2004**, 16, S973-S982	1.8	56
125	Elastic anisotropy of FeSiO3 end-members of the perovskite and post-perovskite phases. *Geophysical Research Letters*, **2006**, 33, n/a-n/a	4.9	55
124	Electronic structure of the antiferromagnetic B1-structured FeO. *Physical Review B*, **2004**, 70,	3.3	53
123	Neutron diffraction at simultaneous high temperatures and pressures, with measurement of temperature by neutron radiography. *Mineralogical Magazine*, **2001**, 65, 737-748	1.7	53
122	A spinel to □phase transformation mechanism in (Mg,Fe)2SiO4. *Nature*, **1982**, 296, 729-731	50.4	52
121	Thermal expansion and atomic displacement parameters of cubic KMgF3perovskite determined by high-resolution neutron powder diffraction. *Journal of Applied Crystallography*, **2002**, 35, 291-295	3.8	51
120	First principles calculations on the diffusivity and viscosity of liquid Fe□ at experimentally accessible conditions. *Physics of the Earth and Planetary Interiors*, **2000**, 120, 145-152	2.3	50
119	High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores. *Earth and Planetary Science Letters*, **2008**, 272, 481-487	5.3	46
118	Molecular Dynamics Simulation of Methanolic and Ethanolic Silica-Based Sol□el Solutions at Ambient Temperature and Pressure. *Journal of Physical Chemistry A*, **2002**, 106, 130-148	2.8	46
117	Oxygen in the Earth's core: a first-principles study. *Physics of the Earth and Planetary Interiors*, **1999**, 110, 191-210	2.3	46
116	Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO3 post-perovskite. *Geophysical Research Letters*, **2006**, 33,	4.9	44
115	CaSiO3 perovskite at lower mantle pressures. *Geophysical Research Letters*, **2005**, 32,	4.9	42

114	Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. *Geophysical Research Letters*, **2005**, 32,	4.9	42
113	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	2.3	40
112	The structure of iron under the conditions of the Earth's inner core. *Geophysical Research Letters*, **1999**, 26, 1231-1234	4.9	40
111	The Grüneisen parameter: computer calculations via lattice dynamics. *Physics of the Earth and Planetary Interiors*, **1994**, 82, 261-270	2.3	39
110	Exsolution microstructures in titanomagnetites and their magnetic significance. *Physics of the Earth and Planetary Interiors*, **1980**, 23, 2-12	2.3	39
109	Elasticity of (Mg, Fe)(Si, Al)O3-perovskite at high pressure. *Earth and Planetary Science Letters*, **2005**, 240, 529-536	5.3	38
108	Computer modelling of B2O3. I. New interatomic potentials, crystalline phases and predicted polymorphs. *Journal of Physics Condensed Matter*, **1995**, 7, 8659-8692	1.8	37
107	Proton-containing defects at forsterite {010} tilt grain boundaries and stepped surfaces. *American Mineralogist*, **2000**, 85, 1143-1154	2.9	36
106	High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al2O3. *Geophysical Research Letters*, **2005**, 32,	4.9	35
105	Primary slip system of iron and anisotropy of the Earth's inner core. *Physics of the Earth and Planetary Interiors*, **1999**, 110, 147-156	2.3	35
104	The nature and significance of stacking faults in wadsleyite, natural (Mg, Fe)2SiO4 from the Peace River meteorite. *Physics of the Earth and Planetary Interiors*, **1983**, 33, 137-147	2.3	35
103	The optical constants of ordinary glass from 0.29 to 4000 cm-1. *Journal Physics D: Applied Physics*, **1975**, 8, 1353-1358	3	34
102	Computer simulation of defects and diffusion in perovskites. *Journal of Geophysical Research*, **1993**, 98, 22245-22253		33
101	Ab initio theory of planetary materials. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2005**, 220,	1	32
100	Ab initio total-energy pseudopotential calculations for polymorphic B2O3 crystals. *Physical Review B*, **1995**, 51, 1447-1455	3.3	32
99	Absolute ionic diffusion in MgO: computer calculations via lattice dynamics. *Physics of the Earth and Planetary Interiors*, **1995**, 88, 193-210	2.3	32
98	High-temperature creep of the perovskites CaTiO3 and NaNbO3. *Physics of the Earth and Planetary Interiors*, **1992**, 74, 9-22	2.3	32
97	Relative stability of zeolite frameworks from calculated energetics of known and theoretical structures. *Zeolites*, **1989**, 9, 321-328		32

96	Thermal expansion of mantle minerals at high pressures: A theoretical study. *Geophysical Research Letters*, **1990**, 17, 689-692	4.9	32
95	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	2.3	31
94	Electronic structure study of the high-pressure vibrational spectrum of FeS2 pyrite. *Journal of Physical Chemistry B*, **2005**, 109, 22067-73	3.4	31
93	Deriving empirical potentials for molecular ionic materials. *Mineralogical Magazine*, **1995**, 59, 617-622	1.7	31
92	Ab initio thermodynamics and phase diagram of solid magnesium: a comparison of the LDA and GGA. *Journal of Chemical Physics*, **2006**, 125, 194507	3.9	30
91	Thermodynamics from first principles: temperature and composition of the Earth's core. *Mineralogical Magazine*, **2003**, 67, 113-123	1.7	30
90	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	2.8	30
89	Computer modelling of B2O3. II. Molecular dynamics simulations of vitreous structures. *Journal of Physics Condensed Matter*, **1995**, 7, 8693-8722	1.8	29
88	The melting of MgO studied by molecular dynamics simulation. *Modelling and Simulation in Materials Science and Engineering*, **1994**, 2, 1101-1110	2	29
87	Ab initio calculations on the free energy and high P-T elasticity of face-centred-cubic iron. *Earth and Planetary Science Letters*, **2008**, 268, 444-449	5.3	28
86	First-principles simulation of high-pressure polymorphs in MgAl2O4. *Physics and Chemistry of Minerals*, **2008**, 35, 381-386	1.6	28
85	The melting curve of iron from quantum mechanics calculations. *Journal of Physics and Chemistry of Solids*, **2004**, 65, 1573-1580	3.9	28
84	Theoretical investigation of metastable Al2SiO5 polymorphs. *Acta Crystallographica Section A: Foundations and Advances*, **2001**, 57, 548-57		28
83	Computer simulation of the MgSiO3 polymorphs. *Physics and Chemistry of Minerals*, **1992**, 18, 365	1.6	28
82	Polytypism and the factors determining the stability of spinelloid structures. *Physics and Chemistry of Minerals*, **1983**, 10, 77-83	1.6	28
81	A computer simulation of the structure and elastic properties of MgSiO3 perovskite. *Mineralogical Magazine*, **1986**, 50, 693-707	1.7	28
80	Elasticity of Mg2SiO4 ringwoodite at mantle conditions. *Physics of the Earth and Planetary Interiors*, **2006**, 157, 181-187	2.3	27
79	A high-pressure study of ?-FeSi, between 0 and 8.5 GPa, by time-of-flight neutron powder diffraction. *Journal of Applied Crystallography*, **1996**, 29, 215-218	3.8	27

78	The factors influencing cation site-preferences in spinels a new mendelyevian approach. *Physics and Chemistry of Minerals*, **1982**, 8, 69-76	1.6	27
77	Computer modelling of a pressure induced phase change in clinoenstatite pyroxenes. *Physics and Chemistry of Minerals*, **1997**, 25, 55-62	1.6	26
76	Structural and magnetic phase transitions in simple oxides using hybrid functionals. *Molecular Simulation*, **2005**, 31, 367-377	2	26
75	Infrared spectroscopy of the polymorphic series (enstatite, ilmenite, and perovskite) of MgSiO3, MgGeO3, and MnGeO3. *Journal of Geophysical Research*, **1989**, 94, 15687-15701		25
74	EVOLUTION AND PALEOGEOGRAPHIC DISTRIBUTION OF THE LEPIDOCYCLINIDS. *Journal of Foraminiferal Research*, **2010**, 40, 79-108	1.1	24
73	Dopant control over the crystal morphology of ceramic materials. *Surface Science*, **2007**, 601, 4793-4800	1.8	24
72	The ab initio simulation of the Earth's core. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2002**, 360, 1227-44	3	24
71	Electrical conductivity of the lower mantle: a molecular dynamics simulation of MgSiO3 perovskite. *Physics of the Earth and Planetary Interiors*, **1989**, 58, 192-204	2.3	24
70	The energetics of polytypic structures: a computer simulation of magnesium silicate spinelloids. *Acta Crystallographica Section B: Structural Science*, **1985**, 41, 231-239		24
69	Crystal structure of tetrapropylammonium fluoride-silicalite. *Nature*, **1981**, 292, 818-819	50.4	24
68	Dislocations in CaTiO3 perovskite deformed at high-temperature: a transmission electron microscopy study. *Physics and Chemistry of Minerals*, **1996**, 23, 337	1.6	23
67	Comparison between the lattice dynamics and molecular dynamics methods: Calculation results for MgSiO3 perovskite. *Geophysical Research Letters*, **1994**, 21, 1659-1662	4.9	23
66	The properties and behaviour of mantle minerals: a computer-simulation approach. *Philosophical Transactions of the Royal Society A*, **1989**, 328, 391-407		22
65	Site preference of vanadium doped into ZrSiO4 and ZrGeO4 and of terbium doped into ZrGeO4. *Journal of the Chemical Society Dalton Transactions*, **1992**, 1579		21
64	Molecular dynamics simulation of polymorphic and polyamorphic transitions in tetrahedral network glasses: BeF2 and GeO2. *Journal of Non-Crystalline Solids*, **2007**, 353, 1892-1898	3.9	20
63	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	2.3	19
62	Molecular dynamics simulation of temperature-induced structural changes in cristobalite, coesite and amorphous silica. *Journal of Non-Crystalline Solids*, **2008**, 354, 181-187	3.9	19
61	Ab initio molecular dynamics simulations for thermal equation of state of B2-type NaCl. *Journal of Applied Physics*, **2008**, 103, 023510	2.5	19

60	Laboratory impact experiments versus natural impact events **2002**,		19
59	A simple, systematic method for the generation periodic, 2-dimensional, 3-connected nets for the description of zeolite frameworks. *Zeolites*, **1992**, 12, 320-327		19
58	Industrial Applications of Simulation Studies in Solid State Chemistry. *Molecular Simulation*, **1989**, 3, 49-69		19
57	Elastic, thermal and structural properties of platinum. *Journal of Physics and Chemistry of Solids*, **2011**, 72, 169-175	3.9	18
56	Ab initio thermodynamics of MgSiO3 perovskite at high pressures and temperatures. *Journal of Chemical Physics*, **2005**, 122, 124501	3.9	18
55	An ab initio study of the relative stabilities and equations of state of FeS polymorphs. *Mineralogical Magazine*, **2001**, 65, 181-191	1.7	18
54	Diffusion in the titanomagnetite solid solution series. *Mineralogical Magazine*, **1981**, 44, 195-200	1.7	18
53	Dispersive Fourier transform measurements on opaque solids from 5 to 350 cm⁻¹. *Infrared Physics*, **1976**, 16, 311-315		18
52	The phylogenetic and palaeogeographic evolution of the miogypsinid larger benthic foraminifera. *Journal of the Geological Society*, **2013**, 170, 185-208	2.7	17
51	Atomistic modeling of silica based sol-gel processes. *Journal of Sol-Gel Science and Technology*, **1997**, 8, 55-58	2.3	17
50	Phase transitions of BaCO3 at high pressures. *Mineralogical Magazine*, **2008**, 72, 659-665	1.7	17
49	Crystal morphology and surface structures of orthorhombic MgSiO3 perovskite. *Physics and Chemistry of Minerals*, **2005**, 31, 671-682	1.6	17
48	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	2.9	17
47	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	1.8	16
46	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	1.8	16
45	Microstructures in titanomagnetites as guides to cooling rates of a Swedish intrusion. *Geological Magazine*, **1979**, 116, 313-318	2	16
44	Structures and physical properties of epsilon-FeSi-type and CsCl-type RuSi studied by first-principles pseudopotential calculations. *Acta Crystallographica Section B: Structural Science*, **2000**, 56 (Pt 3), 369-76		15
43	Thermodynamic Stability of Fe/O Solid Solution at Inner-Core Conditions. *Geophysical Research Letters*, **2000**, 27, 2417-2420	4.9	15

42	Thermodynamic and anharmonic properties of forsterite, □Mg2SiO4: Computer modelling versus high-pressure and high-temperature measurements. *Journal of Geophysical Research*, **1992**, 97, 19791		15
41	The structural relation between svetlozarite and dachiardite. *Mineralogical Magazine*, **1982**, 45, 157-161	1.7	15
40	A Transferable Interatomic Potential for Calcium Carbonate. *Molecular Simulation*, **1992**, 9, 175-177	2	14
39	Computational mineral physics and the physical properties of perovskite. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2002**, 360, 2507-20	3	13
38	Submillimeter-Wave Dielectric Measurements on Absorbing Materials. *IEEE Transactions on Instrumentation and Measurement*, **1974**, 23, 483-488	5.2	13
37	An equilibrium theory of polytypism. *Bulletin De Mineralogie*, **1986**, 109, 3-13		13
36	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	0.7	13
35	Ab initio molecular dynamics study of elasticity of akimotoite MgSiO3 at mantle conditions. *Physics of the Earth and Planetary Interiors*, **2009**, 173, 115-120	2.3	12
34	Thermoelastic properties of magnesiowüstite, (Mg1−xFex)O: determination of the Anderson–Grüneisen parameter by time-of-flight neutron powder diffraction at simultaneous high pressures and temperatures. *Journal of Applied Crystallography*, **2008**, 41, 886-896	3.8	12
33	The effect of cation-ordering on the elastic properties of majorite: An ab initio study. *Earth and Planetary Science Letters*, **2007**, 256, 28-35	5.3	12
32	The nature and significance of exsolved phases in some chrome spinels from the Rhum layered intrusion. *Mineralogical Magazine*, **1979**, 43, 519-526	1.7	12
31	Ab initio molecular dynamic simulation on the elasticity of Mg3Al2Si3O12 pyrope. *Journal of Earth Science (Wuhan, China)*, **2011**, 22, 169-175	2.2	11
30	The energetics of polytypic structures: further applications of the ANNNI model. *Acta Crystallographica Section B: Structural Science*, **1985**, 41, 310-319		11
29	A computer simulation approach to the high pressure thermoelasticity of MgSiO3 perovskite. *Physics of the Earth and Planetary Interiors*, **1996**, 98, 55-63	2.3	10
28	A mechanism for pyroxene-pyroxenoid and pyroxenoid-pyroxenoid transformations. *Physics and Chemistry of Minerals*, **1984**, 10, 236-243	1.6	10
27	Dislocation melting of metals. *Physics of the Earth and Planetary Interiors*, **1992**, 69, 153-162	2.3	9
26	Periodic ab initio Hartree-Fock study of trigonal and orthorhombic phases of boric oxides. *Physics and Chemistry of Minerals*, **1997**, 24, 423-431	1.6	8
25	Structural & physical properties of the binary transition metal- containing perovskite La2CoMnO6. *Synthetic Metals*, **2001**, 121, 1467-1468	3.6	8

24	A microscopic model for a very stable incommensurate modulated mineral: mullite. *Journal of Physics Condensed Matter*, **1993**, 5, 3417-3430	1.8	8
23	The effect of many-body forces on the elastic properties of simple oxides and olivine. *Physics and Chemistry of Minerals*, **1988**, 16, 42	1.6	8
22	Structural phase transitions in IrO2at high pressures. *Journal of Physics Condensed Matter*, **2008**, 20, 045202	2.2	7
21	Ab initio study of the phase separation of argon in molten iron at high pressures. *Geophysical Research Letters*, **2006**, 33,	4.9	7
20	Computer simulations of iron in magnesium silicate perovskite. *Geophysical Research Letters*, **1989**, 16, 1399-1402	4.9	7
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18	A model for polysomatism. *Mineralogical Magazine*, **1986**, 50, 149-156	1.7	7
17	High-temperature structural phase transitions in neighborite: a high-resolution neutron powder diffraction investigation. *Physics and Chemistry of Minerals*, **2015**, 42, 45-52	1.6	6
16	The factors influencing solid state structure A modern Mendeleyevian answer. *Solid State Communications*, **1981**, 40, 923-926	1.6	6
15	Crystal morphology and surface structures of orthorhombic MgSiO3 in the presence of divalent impurity ions. *Physics and Chemistry of Minerals*, **2005**, 32, 379-387	1.6	5
14	A new approach to simulating disorder in crystals. *Physics and Chemistry of Minerals*, **1990**, 17, 238	1.6	5
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12	Molecular dynamics: some recent developments in classical and quantum mechanical simulation of minerals. *Mineralogical Magazine*, **1995**, 59, 597-605	1.7	5
11	The Computer Simulation of the Lattice Dynamics of Silicates **1988**, 591-618		5
10	Defects and diffusion in MgSiO3 perovskite: a computer simulation. *Geophysical Monograph Series*, **2013**, 45-53	1.1	4
9	The eMinerals collaboratory: tools and experience. *Molecular Simulation*, **2005**, 31, 329-337	2	4
8	An ab initio study of the relative stabilities and equations of state of Fe3S polymorphs. *Mineralogical Magazine*, **2004**, 68, 813-817	1.7	4
7	Oxidation phenomena in pleonaste bearing titanomagnetites. *Contributions To Mineralogy and Petrology*, **1979**, 69, 355-359	3.5	4

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