

David Price

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.

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	High-temperature structural phase transitions in neighborite: a high-resolution neutron powder diffraction investigation. <i>Physics and Chemistry of Minerals</i> , 2015 , 42, 45-52	1.6	6
184	Defects and diffusion in MgSiO ₃ perovskite: a computer simulation. <i>Geophysical Monograph Series</i> , 2013 , 45-53	1.1	4
183	The phylogenetic and palaeogeographic evolution of the miogypsinid larger benthic foraminifera. <i>Journal of the Geological Society</i> , 2013 , 170, 185-208	2.7	17
182	Ab initio molecular dynamic simulation on the elasticity of Mg ₃ Al ₂ Si ₃ O ₁₂ pyrope. <i>Journal of Earth Science (Wuhan, China)</i> , 2011 , 22, 169-175	2.2	11
181	Elastic, thermal and structural properties of platinum. <i>Journal of Physics and Chemistry of Solids</i> , 2011 , 72, 169-175	3.9	18
180	EVOLUTION AND PALEOGEOGRAPHIC DISTRIBUTION OF THE LEPIDOCYCLINIDS. <i>Journal of Foraminiferal Research</i> , 2010 , 40, 79-108	1.1	24
179	A computer simulation study of the effect of pressure on Mg diffusion in forsterite. <i>Physics of the Earth and Planetary Interiors</i> , 2009 , 172, 13-19	2.3	19
178	Ab initio molecular dynamics study of elasticity of akimotoite MgSiO ₃ at mantle conditions. <i>Physics of the Earth and Planetary Interiors</i> , 2009 , 173, 115-120	2.3	12
177	Molecular dynamics simulation of temperature-induced structural changes in cristobalite, coesite and amorphous silica. <i>Journal of Non-Crystalline Solids</i> , 2008 , 354, 181-187	3.9	19
176	The stability of bcc-Fe at high pressures and temperatures with respect to tetragonal strain. <i>Physics of the Earth and Planetary Interiors</i> , 2008 , 170, 52-59	2.3	31
175	Ab initio calculations on the free energy and high P-T elasticity of face-centred-cubic iron. <i>Earth and Planetary Science Letters</i> , 2008 , 268, 444-449	5.3	28
174	High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores. <i>Earth and Planetary Science Letters</i> , 2008 , 272, 481-487	5.3	46
173	Ab initio molecular dynamics simulations for thermal equation of state of B2-type NaCl. <i>Journal of Applied Physics</i> , 2008 , 103, 023510	2.5	19
172	Phase transitions of BaCO ₃ at high pressures. <i>Mineralogical Magazine</i> , 2008 , 72, 659-665	1.7	17
171	Structural phase transitions in IrO ₂ at high pressures. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 045202	2.0	7
170	First-principles simulation of high-pressure polymorphs in MgAl ₂ O ₄ . <i>Physics and Chemistry of Minerals</i> , 2008 , 35, 381-386	1.6	28
169	Thermoelastic properties of magnesiowüstite, (Mg _{1-x} Fe _x)O: determination of the Anderson-Grüneisen parameter by time-of-flight neutron powder diffraction at simultaneous high pressures and temperatures. <i>Journal of Applied Crystallography</i> , 2008 , 41, 886-896	3.8	12

168	POWDER NEUTRON-DIFFRACTION STUDIES OF CLINOPYROXENES. I. THE CRYSTAL STRUCTURE AND THERMOELASTIC PROPERTIES OF JADEITE BETWEEN 1.5 AND 270 K. <i>Canadian Mineralogist</i> , 2008 , 46, 1593-1622	0.7	13
167	Dopant control over the crystal morphology of ceramic materials. <i>Surface Science</i> , 2007 , 601, 4793-4800	1.8	24
166	Electronic spin transitions in iron-bearing MgSiO ₃ perovskite. <i>Earth and Planetary Science Letters</i> , 2007 , 253, 282-290	5.3	89
165	The effect of cation-ordering on the elastic properties of majorite: An ab initio study. <i>Earth and Planetary Science Letters</i> , 2007 , 256, 28-35	5.3	12
164	Molecular dynamics simulation of polymorphic and polyamorphic transitions in tetrahedral network glasses: BeF ₂ and GeO ₂ . <i>Journal of Non-Crystalline Solids</i> , 2007 , 353, 1892-1898	3.9	20
163	Temperature and composition of the Earth's core. <i>Contemporary Physics</i> , 2007 , 48, 63-80	3.3	67
162	Elastic anisotropy of FeSiO ₃ end-members of the perovskite and post-perovskite phases. <i>Geophysical Research Letters</i> , 2006 , 33, n/a-n/a	4.9	55
161	Ab initio study of the phase separation of argon in molten iron at high pressures. <i>Geophysical Research Letters</i> , 2006 , 33,	4.9	7
160	Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO ₃ post-perovskite. <i>Geophysical Research Letters</i> , 2006 , 33,	4.9	44
159	First-principles modelling of Earth and planetary materials at high pressures and temperatures. <i>Reports on Progress in Physics</i> , 2006 , 69, 2365-2441	14.4	133
158	Elasticity of CaSiO ₃ perovskite at high pressure and high temperature. <i>Physics of the Earth and Planetary Interiors</i> , 2006 , 155, 249-259	2.3	72
157	Phase stability of CaSiO ₃ perovskite at high pressure and temperature: Insights from ab initio molecular dynamics. <i>Physics of the Earth and Planetary Interiors</i> , 2006 , 155, 260-268	2.3	40
156	Elasticity of Mg ₂ SiO ₄ ringwoodite at mantle conditions. <i>Physics of the Earth and Planetary Interiors</i> , 2006 , 157, 181-187	2.3	27
155	Ab initio thermodynamics and phase diagram of solid magnesium: a comparison of the LDA and GGA. <i>Journal of Chemical Physics</i> , 2006 , 125, 194507	3.9	30
154	The eMinerals collaboratory: tools and experience. <i>Molecular Simulation</i> , 2005 , 31, 329-337	2	4
153	Ab initio thermodynamics of MgSiO ₃ perovskite at high pressures and temperatures. <i>Journal of Chemical Physics</i> , 2005 , 122, 124501	3.9	18
152	Structural and magnetic phase transitions in simple oxides using hybrid functionals. <i>Molecular Simulation</i> , 2005 , 31, 367-377	2	26
151	Ab initio theory of planetary materials. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2005 , 220,	1	32

150	The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO ₃ . <i>Earth and Planetary Science Letters</i> , 2005 , 230, 1-10	5.3	129
149	Elasticity of (Mg, Fe)(Si, Al)O ₃ -perovskite at high pressure. <i>Earth and Planetary Science Letters</i> , 2005 , 240, 529-536	5.3	38
148	CaSiO ₃ perovskite at lower mantle pressures. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	42
147	Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	42
146	High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al ₂ O ₃ . <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	35
145	Electronic structure study of the high-pressure vibrational spectrum of FeS ₂ pyrite. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 22067-73	3.4	31
144	Structural stability of silica at high pressures and temperatures. <i>Physical Review B</i> , 2005 , 71,	3.3	121
143	Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. <i>Nature</i> , 2005 , 438, 1004-7	50.4	175
142	Crystal morphology and surface structures of orthorhombic MgSiO ₃ perovskite. <i>Physics and Chemistry of Minerals</i> , 2005 , 31, 671-682	1.6	17
141	Crystal morphology and surface structures of orthorhombic MgSiO ₃ in the presence of divalent impurity ions. <i>Physics and Chemistry of Minerals</i> , 2005 , 32, 379-387	1.6	5
140	An ab initio study of the relative stabilities and equations of state of Fe ₃ S polymorphs. <i>Mineralogical Magazine</i> , 2004 , 68, 813-817	1.7	4
139	Electronic structure of the antiferromagnetic B1-structured FeO. <i>Physical Review B</i> , 2004 , 70,	3.3	53
138	The influence of potassium on core and geodynamo evolution. <i>Geophysical Journal International</i> , 2004 , 156, 363-376	2.6	152
137	Gross thermodynamics of two-component core convection. <i>Geophysical Journal International</i> , 2004 , 157, 1407-1414	2.6	116
136	Thermal expansion and crystal structure of cementite, Fe ₃ C, between 4 and 600 K determined by time-of-flight neutron powder diffraction. <i>Journal of Applied Crystallography</i> , 2004 , 37, 82-90	3.8	153
135	The melting curve of iron from quantum mechanics calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2004 , 65, 1573-1580	3.9	28
134	Molecular dynamics simulations of vitreous silica structures. <i>Journal of Non-Crystalline Solids</i> , 2004 , 345-346, 224-229	3.9	71
133	Melting curve of materials: theory versus experiments. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, S973-S982	1.8	56

132	Can the Earth's dynamo run on heat alone?. <i>Geophysical Journal International</i> , 2003 , 155, 609-622	2.6	108
131	Possible thermal and chemical stabilization of body-centred-cubic iron in the Earth's core. <i>Nature</i> , 2003 , 424, 536-9	50.4	219
130	Thermodynamics from first principles: temperature and composition of the Earth's core. <i>Mineralogical Magazine</i> , 2003 , 67, 113-123	1.7	30
129	Ab initio lattice dynamics and structural stability of MgO. <i>Journal of Chemical Physics</i> , 2003 , 118, 10174-10182	5.82	130
128	The properties of iron under core conditions from first principles calculations. <i>Physics of the Earth and Planetary Interiors</i> , 2003 , 140, 101-125	2.3	126
127	Thermal expansion and crystal structure of FeSi between 4 and 1173 K determined by time-of-flight neutron powder diffraction. <i>Physics and Chemistry of Minerals</i> , 2002 , 29, 132-139	1.6	88
126	Thermal expansion and atomic displacement parameters of cubic KMgF ₃ perovskite determined by high-resolution neutron powder diffraction. <i>Journal of Applied Crystallography</i> , 2002 , 35, 291-295	3.8	51
125	Computational mineral physics and the physical properties of perovskite. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2002 , 360, 2507-20	3	13
124	Molecular Dynamics Simulation of Methanolic and Ethanolic Silica-Based Sol-Gel Solutions at Ambient Temperature and Pressure. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 130-148	2.8	46
123	The ab initio simulation of the Earth's core. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2002 , 360, 1227-44	3	24
122	Complementary approaches to the ab initio calculation of melting properties. <i>Journal of Chemical Physics</i> , 2002 , 116, 6170-6177	3.9	77
121	Composition and temperature of the Earth's core constrained by combining ab initio calculations and seismic data. <i>Earth and Planetary Science Letters</i> , 2002 , 195, 91-98	5.3	221
120	Impact induced melting and the development of large igneous provinces. <i>Earth and Planetary Science Letters</i> , 2002 , 202, 551-561	5.3	100
119	The effect of ferromagnetism on the equation of state of Fe ₃ C studied by first-principles calculations. <i>Earth and Planetary Science Letters</i> , 2002 , 203, 567-575	5.3	102
118	Iron under Earth's core conditions: Liquid-state thermodynamics and high-pressure melting curve from ab initio calculations. <i>Physical Review B</i> , 2002 , 65,	3.3	242
117	Laboratory impact experiments versus natural impact events 2002 ,		19
116	Ab initio chemical potentials of solid and liquid solutions and the chemistry of the Earth's core. <i>Journal of Chemical Physics</i> , 2002 , 116, 7127-7136	3.9	92
115	Theoretical investigation of metastable Al ₂ SiO ₅ polymorphs. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2001 , 57, 548-57		28

114	Thermodynamics of hexagonal-close-packed iron under Earth's core conditions. <i>Physical Review B</i> , 2001 , 64,	3.3	230
113	The elastic constants of MgSiO ₃ perovskite at pressures and temperatures of the Earth's mantle. <i>Nature</i> , 2001 , 411, 934-7	50.4	172
112	An ab initio study of the relative stabilities and equations of state of FeS polymorphs. <i>Mineralogical Magazine</i> , 2001 , 65, 181-191	1.7	18
111	Neutron diffraction at simultaneous high temperatures and pressures, with measurement of temperature by neutron radiography. <i>Mineralogical Magazine</i> , 2001 , 65, 737-748	1.7	53
110	Phonon density of states of iron up to 153 gigapascals. <i>Science</i> , 2001 , 292, 914-6	33.3	264
109	Structural & physical properties of the binary transition metal- containing perovskite La ₂ CoMnO ₆ . <i>Synthetic Metals</i> , 2001 , 121, 1467-1468	3.6	8
108	Ab initio elasticity and thermal equation of state of MgSiO ₃ perovskite. <i>Earth and Planetary Science Letters</i> , 2001 , 184, 555-560	5.3	125
107	Molecular Dynamics Simulation of Liquid H ₂ O, MeOH, EtOH, Si(OMe) ₄ , and Si(OEt) ₄ , as a Function of Temperature and Pressure. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 1909-1925	2.8	30
106	Proton-containing defects at forsterite {010} tilt grain boundaries and stepped surfaces. <i>American Mineralogist</i> , 2000 , 85, 1143-1154	2.9	36
105	Structures and physical properties of epsilon-FeSi-type and CsCl-type RuSi studied by first-principles pseudopotential calculations. <i>Acta Crystallographica Section B: Structural Science</i> , 2000 , 56 (Pt 3), 369-76		15
104	Constraints on the composition of the Earth's core from ab initio calculations. <i>Nature</i> , 2000 , 405, 172-5	50.4	88
103	Modelling the effect of water on the surface structure and stability of forsterite. <i>Physics and Chemistry of Minerals</i> , 2000 , 27, 332-341	1.6	93
102	First principles calculations on the diffusivity and viscosity of liquid Fe at experimentally accessible conditions. <i>Physics of the Earth and Planetary Interiors</i> , 2000 , 120, 145-152	2.3	50
101	Comparative study of quasiharmonic lattice dynamics, molecular dynamics and Debye model applied to MgSiO ₃ perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 2000 , 122, 277-288	2.3	97
100	Ab initio free energy calculations on the polymorphs of iron at core conditions. <i>Physics of the Earth and Planetary Interiors</i> , 2000 , 117, 123-137	2.3	79
99	The composition and geotherm of the lower mantle: constraints from the elasticity of silicate perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 2000 , 118, 103-109	2.3	58
98	Thermodynamic Stability of Fe/O Solid Solution at Inner-Core Conditions. <i>Geophysical Research Letters</i> , 2000 , 27, 2417-2420	4.9	15
97	Crystal structure, compressibility and possible phase transitions in boldvarepsilon-FeSi studied by first-principles pseudopotential calculations. <i>Acta Crystallographica Section B: Structural Science</i> , 1999 , 55, 484-493		90

96	The melting curve of iron at the pressures of the Earth's core from ab initio calculations. <i>Nature</i> , 1999 , 401, 462-464	50.4	248
95	Ab Initio Studies of Silica-Based Clusters. Part II. Structures and Energies of Complex Clusters. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 3268-3284	2.8	92
94	Primary slip system of Iron and anisotropy of the Earth's inner core. <i>Physics of the Earth and Planetary Interiors</i> , 1999 , 110, 147-156	2.3	35
93	Oxygen in the Earth's core: a first-principles study. <i>Physics of the Earth and Planetary Interiors</i> , 1999 , 110, 191-210	2.3	46
92	Ab Initio Studies of Silica-Based Clusters. Part I. Energies and Conformations of Simple Clusters. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 3252-3267	2.8	103
91	The structure of iron under the conditions of the Earth's inner core. <i>Geophysical Research Letters</i> , 1999 , 26, 1231-1234	4.9	40
90	The viscosity of liquid iron at the physical conditions of the Earth's core. <i>Nature</i> , 1998 , 392, 805-807	50.4	232
89	Silica condensation reaction: an ab initio study. <i>Chemical Communications</i> , 1998 , 1387-1388	5.8	63
88	Computer simulation of the infrared and Raman activity of pyrope garnet, and assignment of calculated modes to specific atomic motions. <i>American Mineralogist</i> , 1998 , 83, 841-847	2.9	17
87	The influence of thermal vibrations on the average structure of cubic perovskite: a combined molecular dynamics and neutron diffraction study. <i>Journal of Physics Condensed Matter</i> , 1997 , 9, L647-L655	1.8	16
86	First principles calculations on crystalline and liquid iron at Earth's core conditions. <i>Faraday Discussions</i> , 1997 , 106, 205-218	3.6	94
85	Equation of state of MgSiO ₃ -perovskite and MgO (periclase) from computer simulations [discussion. <i>Physics of the Earth and Planetary Interiors</i> , 1997 , 102, 291-292	2.3	
84	Atomistic modeling of silica based sol-gel processes. <i>Journal of Sol-Gel Science and Technology</i> , 1997 , 8, 55-58	2.3	17
83	Periodic ab initio Hartree-Fock study of trigonal and orthorhombic phases of boric oxides. <i>Physics and Chemistry of Minerals</i> , 1997 , 24, 423-431	1.6	8
82	Computer modelling of a pressure induced phase change in clinoenstatite pyroxenes. <i>Physics and Chemistry of Minerals</i> , 1997 , 25, 55-62	1.6	26
81	Dislocations in CaTiO ₃ perovskite deformed at high-temperature: a transmission electron microscopy study. <i>Physics and Chemistry of Minerals</i> , 1996 , 23, 337	1.6	23
80	The melting of MgO [computer calculations via molecular dynamics. <i>Physics and Chemistry of Minerals</i> , 1996 , 23, 42-49	1.6	58
79	A computer simulation approach to the high pressure thermoelasticity of MgSiO ₃ perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 1996 , 98, 55-63	2.3	10

78	A high-pressure study of γ -FeSi, between 0 and 8.5 GPa, by time-of-flight neutron powder diffraction. <i>Journal of Applied Crystallography</i> , 1996 , 29, 215-218	3.8	27
77	Atomistic potentials for MgSiO ₃ with the orthorhombic perovskite structure. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1996 , 73, 41-48		2
76	Deriving empirical potentials for molecular ionic materials. <i>Mineralogical Magazine</i> , 1995 , 59, 617-622	1.7	31
75	Ab initio total-energy pseudopotential calculations for polymorphic B ₂ O ₃ crystals. <i>Physical Review B</i> , 1995 , 51, 1447-1455	3.3	32
74	Computer modelling of B ₂ O ₃ . II. Molecular dynamics simulations of vitreous structures. <i>Journal of Physics Condensed Matter</i> , 1995 , 7, 8693-8722	1.8	29
73	Compressibility of FeSi between 0 and 9 GPa, determined by high pressure time-of-flight neutron powder diffraction. <i>Journal of Physics Condensed Matter</i> , 1995 , 7, L475-L479	1.8	16
72	Absolute ionic diffusion in MgO—computer calculations via lattice dynamics. <i>Physics of the Earth and Planetary Interiors</i> , 1995 , 88, 193-210	2.3	32
71	Ab initio study of MgSiO ₃ and CaSiO ₃ perovskites at lower-mantle pressures. <i>Physics of the Earth and Planetary Interiors</i> , 1995 , 90, 101-112	2.3	149
70	Fe-Mg interdiffusion in olivine up to 9 GPa at T = 600–800°C; experimental data and comparison with defect calculations. <i>Physics of the Earth and Planetary Interiors</i> , 1995 , 89, 199-218	2.3	65
69	Molecular dynamics simulations of CaCO ₃ melts to mantle pressures and temperatures: implications for carbonatite magmas. <i>Earth and Planetary Science Letters</i> , 1995 , 131, 225-238	5.3	80
68	Computer modelling of B ₂ O ₃ . I. New interatomic potentials, crystalline phases and predicted polymorphs. <i>Journal of Physics Condensed Matter</i> , 1995 , 7, 8659-8692	1.8	37
67	An infrared and Raman study of carbonate glasses: implications for the structure of carbonatite magmas. <i>Geochimica Et Cosmochimica Acta</i> , 1995 , 59, 927-937	5.5	83
66	Molecular dynamics: some recent developments in classical and quantum mechanical simulation of minerals. <i>Mineralogical Magazine</i> , 1995 , 59, 597-605	1.7	5
65	The melting of MgO studied by molecular dynamics simulation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 1994 , 2, 1101-1110	2	29
64	Comparison between the lattice dynamics and molecular dynamics methods: Calculation results for MgSiO ₃ perovskite. <i>Geophysical Research Letters</i> , 1994 , 21, 1659-1662	4.9	23
63	The Grüneisen parameter—computer calculations via lattice dynamics. <i>Physics of the Earth and Planetary Interiors</i> , 1994 , 82, 261-270	2.3	39
62	Ab initio molecular dynamics with variable cell shape: Application to MgSiO ₃ . <i>Physical Review Letters</i> , 1993 , 70, 3947-3950	7.4	247
61	Computer simulation of defects and diffusion in perovskites. <i>Journal of Geophysical Research</i> , 1993 , 98, 22245-22253		33

60	A microscopic model for a very stable incommensurate modulated mineral: mullite. <i>Journal of Physics Condensed Matter</i> , 1993 , 5, 3417-3430	1.8	8
59	Comparative study of all-electron and core pseudo-potentials basis sets for periodic AB INITIO hartree-fock calculation: The case of MgSiO ₃ -ilmenite. <i>Journal of Physics and Chemistry of Solids</i> , 1993 , 54, 281-287	3.9	3
58	Phase changes and thermodynamic properties of CaTiO ₃ . Spectroscopic data, vibrational modelling and some insights on the properties of MgSiO ₃ perovskite. <i>Physics and Chemistry of Minerals</i> , 1993 , 20, 159-170	1.6	62
57	The stability of minerals: an introduction 1992 , 1-24		
56	A Transferable Interatomic Potential for Calcium Carbonate. <i>Molecular Simulation</i> , 1992 , 9, 175-177	2	14
55	Site preference of vanadium doped into ZrSiO ₄ and ZrGeO ₄ and of terbium doped into ZrGeO ₄ . <i>Journal of the Chemical Society Dalton Transactions</i> , 1992 , 1579		21
54	Thermodynamic and anharmonic properties of forsterite, Mg ₂ SiO ₄ : Computer modelling versus high-pressure and high-temperature measurements. <i>Journal of Geophysical Research</i> , 1992 , 97, 19791		15
53	High-temperature creep of the perovskites CaTiO ₃ and NaNbO ₃ . <i>Physics of the Earth and Planetary Interiors</i> , 1992 , 74, 9-22	2.3	32
52	Dislocation melting of metals. <i>Physics of the Earth and Planetary Interiors</i> , 1992 , 69, 153-162	2.3	9
51	Interatomic potentials for CaCO ₃ polymorphs (calcite and aragonite), fitted to elastic and vibrational data. <i>Physics and Chemistry of Minerals</i> , 1992 , 19, 80	1.6	96
50	Computer simulation of the MgSiO ₃ polymorphs. <i>Physics and Chemistry of Minerals</i> , 1992 , 18, 365	1.6	28
49	A simple, systematic method for the generation periodic, 2-dimensional, 3-connected nets for the description of zeolite frameworks. <i>Zeolites</i> , 1992 , 12, 320-327		19
48	Simulation of the pre-melting behaviour of MgSiO ₃ perovskite at high pressures and temperatures. <i>Nature</i> , 1991 , 351, 735-737	50.4	99
47	Reply [to Comment on Infrared spectroscopy of the polymorphic series (enstatite, ilmenite, and perovskite) of MgSiO ₃ , MgGeO ₃ , and MnGeO ₃] by Michel Madon and Geoffrey D. Price] <i>Journal of Geophysical Research</i> , 1991 , 96, 21965-21965		
46	Computer modelling of solid-state inorganic materials. <i>Nature</i> , 1990 , 347, 243-248	50.4	127
45	A new approach to simulating disorder in crystals. <i>Physics and Chemistry of Minerals</i> , 1990 , 17, 238	1.6	5
44	Thermal expansion of mantle minerals at high pressures: A theoretical study. <i>Geophysical Research Letters</i> , 1990 , 17, 689-692	4.9	32
43	The properties and behaviour of mantle minerals: a computer-simulation approach. <i>Philosophical Transactions of the Royal Society A</i> , 1989 , 328, 391-407		22

42	Relative stability of zeolite frameworks from calculated energetics of known and theoretical structures. <i>Zeolites</i> , 1989 , 9, 321-328		32
41	Systematic enumeration of zeolite frameworks. <i>Zeolites</i> , 1989 , 9, 23-32		64
40	Computer simulations of iron in magnesium silicate perovskite. <i>Geophysical Research Letters</i> , 1989 , 16, 1399-1402	4.9	7
39	Industrial Applications of Simulation Studies in Solid State Chemistry. <i>Molecular Simulation</i> , 1989 , 3, 49-69		19
38	Electrical conductivity of the lower mantle: a molecular dynamics simulation of MgSiO ₃ perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 1989 , 58, 192-204	2.3	24
37	Infrared spectroscopy of the polymorphic series (enstatite, ilmenite, and perovskite) of MgSiO ₃ , MgGeO ₃ , and MnGeO ₃ . <i>Journal of Geophysical Research</i> , 1989 , 94, 15687-15701		25
36	The effect of many-body forces on the elastic properties of simple oxides and olivine. <i>Physics and Chemistry of Minerals</i> , 1988 , 16, 42	1.6	8
35	Gravity glide and plate tectonics. <i>Geological Society Special Publication</i> , 1988 , 37, 5-21	1.7	3
34	The Computer Simulation of the Lattice Dynamics of Silicates 1988 , 591-618		5
33	The lattice dynamics of forsterite. <i>Mineralogical Magazine</i> , 1987 , 51, 157-170	1.7	74
32	The lattice dynamics and thermodynamics of the Mg ₂ SiO ₄ polymorphs. <i>Physics and Chemistry of Minerals</i> , 1987 , 15, 181-190	1.6	100
31	A computer simulation of the structure and elastic properties of MgSiO ₃ perovskite. <i>Mineralogical Magazine</i> , 1986 , 50, 693-707	1.7	28
30	A model for polysomatism. <i>Mineralogical Magazine</i> , 1986 , 50, 149-156	1.7	7
29	An equilibrium theory of polytypism. <i>Bulletin De Mineralogie</i> , 1986 , 109, 3-13		13
28	A study of the structures and energetics of magnesium silicates. <i>Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics</i> , 1985 , 131, 290-299		7
27	The energetics of polytypic structures: a computer simulation of magnesium silicate spinelloids. <i>Acta Crystallographica Section B: Structural Science</i> , 1985 , 41, 231-239		24
26	The energetics of polytypic structures: further applications of the ANNNI model. <i>Acta Crystallographica Section B: Structural Science</i> , 1985 , 41, 310-319		11
25	Computer simulations of the structural and physical properties of the olivine and spinel polymorphs of Mg ₂ SiO ₄ . <i>Physics and Chemistry of Minerals</i> , 1984 , 10, 209-216	1.6	93

24	A mechanism for pyroxene-pyroxenoid and pyroxenoid-pyroxenoid transformations. <i>Physics and Chemistry of Minerals</i> , 1984 , 10, 236-243	1.6	10
23	The application of the ANNNI model to polytypic behaviour. <i>Acta Crystallographica Section B: Structural Science</i> , 1984 , 40, 448-454		66
22	Synthesis of 1,4-dinitrocubane. <i>Journal of Organic Chemistry</i> , 1984 , 49, 185-186	4.2	79
21	Polytypism and the factors determining the stability of spinelloid structures. <i>Physics and Chemistry of Minerals</i> , 1983 , 10, 77-83	1.6	28
20	The nature and significance of stacking faults in wadsleyite, natural $\text{[(Mg, Fe)}_2\text{SiO}_4$ from the Peace River meteorite. <i>Physics of the Earth and Planetary Interiors</i> , 1983 , 33, 137-147	2.3	35
19	The structural relation between svetlozarite and dachiardite. <i>Mineralogical Magazine</i> , 1982 , 45, 157-161	1.7	15
18	Exsolution in titanomagnetites as an indicator of cooling rates. <i>Mineralogical Magazine</i> , 1982 , 46, 19-25	1.7	5
17	Crystal structure of tetrapropylammonium fluoride-containing precursor to fluoride silicalite. <i>Journal of the American Chemical Society</i> , 1982 , 104, 5971-5977	16.4	136
16	Role of the crystal-field theory in determining the structures of spinels. <i>Journal of the American Chemical Society</i> , 1982 , 104, 92-95	16.4	138
15	The factors influencing cation site-preferences in spinels a new mendelyevian approach. <i>Physics and Chemistry of Minerals</i> , 1982 , 8, 69-76	1.6	27
14	A spinel to β phase transformation mechanism in $(\text{Mg,Fe})_2\text{SiO}_4$. <i>Nature</i> , 1982 , 296, 729-731	50.4	52
13	Factors influencing solid-state structure—an analysis using pseudopotential radii structural maps. <i>Physical Review B</i> , 1981 , 24, 2903-2912	3.3	62
12	Diffusion in the titanomagnetite solid solution series. <i>Mineralogical Magazine</i> , 1981 , 44, 195-200	1.7	18
11	Crystal structure of tetrapropylammonium fluoride-silicalite. <i>Nature</i> , 1981 , 292, 818-819	50.4	24
10	The factors influencing solid state structure—a modern Mendeleevian answer. <i>Solid State Communications</i> , 1981 , 40, 923-926	1.6	6
9	Exsolution microstructures in titanomagnetites and their magnetic significance. <i>Physics of the Earth and Planetary Interiors</i> , 1980 , 23, 2-12	2.3	39
8	Electron petrography of shock-produced veins in the Tenham chondrite. <i>Contributions To Mineralogy and Petrology</i> , 1979 , 71, 211-218	3.5	91
7	Oxidation phenomena in pleonaste bearing titanomagnetites. <i>Contributions To Mineralogy and Petrology</i> , 1979 , 69, 355-359	3.5	4

6	High-pressure (Mg, Fe) ₂ SiO ₄ phases in the Tenham chondritic meteorite. <i>Nature</i> , 1979 , 280, 217-218	50.4	89
5	The nature and significance of exsolved phases in some chrome spinels from the Rhum layered intrusion. <i>Mineralogical Magazine</i> , 1979 , 43, 519-526	1.7	12
4	Microstructures in titanomagnetites as guides to cooling rates of a Swedish intrusion. <i>Geological Magazine</i> , 1979 , 116, 313-318	2	16
3	Dispersive Fourier transform measurements on opaque solids from 5 to 350 cm ⁻¹ . <i>Infrared Physics</i> , 1976 , 16, 311-315		18
2	The optical constants of ordinary glass from 0.29 to 4000 cm ⁻¹ . <i>Journal Physics D: Applied Physics</i> , 1975 , 8, 1353-1358	3	34
1	Submillimeter-Wave Dielectric Measurements on Absorbing Materials. <i>IEEE Transactions on Instrumentation and Measurement</i> , 1974 , 23, 483-488	5.2	13