

J P Brodholt

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178
papers

6,849
citations

46
h-index

74
g-index

187
ext. papers

7,417
ext. citations

7.1
avg, IF

5.95
L-index

#	Paper	IF	Citations
178	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
177	First-principles constraints on diffusion in lower-mantle minerals and a weak D'' layer. <i>Nature</i> , 2010 , 465, 462-5	50.4	181
176	Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. <i>Nature</i> , 2005 , 438, 1004-7	50.4	175
175	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
174	A seismologically consistent compositional model of Earth's core. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 7542-5	11.5	167
173	Analysis of the hydrogen-bonded structure of water from ambient to supercritical conditions. <i>Journal of Chemical Physics</i> , 1998 , 108, 8528-8540	3.9	165
172	Two-electron dissociation of single molecules by atomic manipulation at room temperature. <i>Nature</i> , 2005 , 434, 367-71	50.4	161
171	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
170	The influence of potassium on core and geodynamo evolution. <i>Geophysical Journal International</i> , 2004 , 156, 363-376	2.6	152
169	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
168	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
167	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
166	Subducted banded iron formations as a source of ultralow-velocity zones at the core-mantle boundary. <i>Nature</i> , 2005 , 434, 371-4	50.4	124
165	Pressure-induced changes in the compression mechanism of aluminous perovskite in the Earth's mantle. <i>Nature</i> , 2000 , 407, 620-2	50.4	124
164	Arsenic incorporation into FeS ₂ pyrite and its influence on dissolution: A DFT study. <i>Geochimica Et Cosmochimica Acta</i> , 2007 , 71, 624-630	5.5	117
163	Parameterizing a polarizable intermolecular potential for water. <i>Molecular Physics</i> , 1995 , 86, 149-158	1.7	109
162	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

161	Mantle dynamics in super-Earths: Post-perovskite rheology and self-regulation of viscosity. <i>Icarus</i> , 2013 , 225, 50-61	3.8	101
160	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
159	Core formation and core composition from coupled geochemical and geophysical constraints. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 12310-4	11.5	94
158	Simulations of the structure and thermodynamic properties of water at high pressures and temperatures. <i>Journal of Geophysical Research</i> , 1993 , 98, 519-536		91
157	Electronic spin transitions in iron-bearing MgSiO ₃ perovskite. <i>Earth and Planetary Science Letters</i> , 2007 , 253, 282-290	5.3	89
156	Molecular dynamics simulations of aqueous NaCl solutions at high pressures and temperatures. <i>Chemical Geology</i> , 1998 , 151, 11-19	4.2	85
155	A test of alternative Caribbean Plate relative motion models. <i>Journal of Geophysical Research</i> , 1988 , 93, 3041		82
154	Strong premelting effect in the elastic properties of hcp-Fe under inner-core conditions. <i>Science</i> , 2013 , 342, 466-8	33.3	81
153	In situ measurement of viscosity of liquids in the Fe-FeS system at high pressures and temperatures. <i>American Mineralogist</i> , 2000 , 85, 1838-1842	2.9	81
152	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
151	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
150	Carbon fluid equilibria and the oxidation state of the upper mantle. <i>Nature</i> , 1991 , 349, 321-324	50.4	70
149	Weakening of calcium iridate during its transformation from perovskite to post-perovskite. <i>Nature Geoscience</i> , 2009 , 2, 794-797	18.3	66
148	The long-term stability of a possible aqueous ammonium sulfate ocean inside Titan. <i>Icarus</i> , 2008 , 197, 137-151	3.8	66
147	Phase relations and equation-of-state of aluminous Mg-silicate perovskite and implications for Earth's lower mantle. <i>Earth and Planetary Science Letters</i> , 2004 , 222, 501-516	5.3	65
146	An ab initio study of hydrogen in forsterite and a possible mechanism for hydrolytic weakening. <i>Journal of Geophysical Research</i> , 2000 , 105, 18977-18982		65
145	The electrical conductivity of the lower mantle phase magnesiowüstite at high temperatures and pressures. <i>Journal of Geophysical Research</i> , 2000 , 105, 531-538		63
144	Ab initio calculations on point defects in forsterite (Mg ₂ SiO ₄) and implications for diffusion and creep. <i>American Mineralogist</i> , 1997 , 82, 1049-1053	2.9	58

143	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
142	Quantum Monte Carlo calculations of the structural properties and the B1-B2 phase transition of MgO. <i>Physical Review B</i> , 2005 , 72,	3.3	53
141	Electronic structure of the antiferromagnetic B1-structured FeO. <i>Physical Review B</i> , 2004 , 70,	3.3	53
140	A High-Temperature Electrical Conduction Mechanism in the Lower Mantle Phase (Mg,Fe) _{1-x} O. <i>Science</i> , 1997 , 275, 1779-81	33.3	52
139	Calculated role of aluminum in the incorporation of ferric iron into magnesium silicate perovskite. <i>American Mineralogist</i> , 1998 , 83, 947-951	2.9	51
138	Elastic properties of MgSiO ₃ -perovskite under lower mantle conditions and the composition of the deep Earth. <i>Earth and Planetary Science Letters</i> , 2013 , 379, 1-12	5.3	50
137	Measurements of the PVT properties of water to 25 kbars and 1600°C from synthetic fluid inclusions in corundum. <i>Geochimica Et Cosmochimica Acta</i> , 1994 , 58, 2143-2148	5.5	50
136	Analysis of the velocity autocorrelation function of water. <i>Journal of Physics Condensed Matter</i> , 1996 , 8, 6139-6144	1.8	48
135	The effect of nickel on the properties of iron at the conditions of Earth's inner core: Ab initio calculations of seismic wave velocities of FeNi alloys. <i>Earth and Planetary Science Letters</i> , 2013 , 365, 143-151	5.3	47
134	Molecular dynamics of water at high temperatures and pressures. <i>Geochimica Et Cosmochimica Acta</i> , 1990 , 54, 2611-2616	5.5	47
133	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
132	Viscosity of liquid water from computer simulations with a polarizable potential model. <i>Physical Review E</i> , 2000 , 62, 2971-3	2.4	46
131	High-pressure phases in the Al ₂ SiO ₅ system and the problem of aluminous phase in the Earth's lower mantle: ab initio calculations. <i>Physics and Chemistry of Minerals</i> , 2000 , 27, 430-439	1.6	45
130	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
129	Hydrogen bonding in solid ammonia from ab initio calculations. <i>Journal of Chemical Physics</i> , 2003 , 118, 5987-5994	3.9	44
128	Relationship of deep seismicity to the thermal structure of subducted lithosphere. <i>Nature</i> , 1991 , 353, 252-255	50.4	43
127	CaSiO ₃ perovskite at lower mantle pressures. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	42
126	Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	42

125	Chemical versus thermal heterogeneity in the lower mantle: The most likely role of anelasticity. <i>Earth and Planetary Science Letters</i> , 2007 , 262, 429-437	5.3	41
124	Ab initio simulation of ammonia monohydrate (NH ₃ ·H ₂ O) and ammonium hydroxide (NH ₄ OH). <i>Journal of Chemical Physics</i> , 2001 , 115, 7006-7014	3.9	41
123	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
122	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
121	Composition of the low seismic velocity E' layer at the top of Earth's core. <i>Geophysical Research Letters</i> , 2017 , 44, 8303-8310	4.9	39
120	The elastic properties of hcp-Fe alloys under the conditions of the Earth's inner core. <i>Earth and Planetary Science Letters</i> , 2018 , 493, 118-127	5.3	38
119	DFT study of migration enthalpies in MgSiO ₃ perovskite. <i>Physics and Chemistry of Minerals</i> , 2009 , 36, 151-158	1.6	38
118	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
117	Variation of thermal conductivity and heat flux at the Earth's core mantle boundary. <i>Earth and Planetary Science Letters</i> , 2014 , 390, 175-185	5.3	37
116	Global systematics of unaveraged mid-ocean ridge basalt compositions: Comment [on Global correlations of ocean ridge basalt chemistry with axial depth and crustal thickness by E. M. Klein and C. H. Langmuir]. <i>Journal of Geophysical Research</i> , 1989 , 94, 4231-4239		37
115	The incorporation of water into lower-mantle perovskites: A first-principles study. <i>Earth and Planetary Science Letters</i> , 2013 , 364, 37-43	5.3	36
114	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
113	Hydration of Sr ²⁺ in Hydrothermal Solutions from ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 9056-9058	3.4	35
112	Light elements in the core: Effects of impurities on the phase diagram of iron. <i>Geophysical Research Letters</i> , 2008 , 35,	4.9	33
111	Unsolved problems in the lowermost mantle. <i>Geophysical Research Letters</i> , 2006 , 33,	4.9	33
110	A high-resolution neutron powder diffraction study of ammonia dihydrate (ND ₃ ·2D ₂ O) phase I. <i>Journal of Chemical Physics</i> , 2003 , 119, 10806-10813	3.9	33
109	Molecular Dynamics simulation of aqueous ZnCl ₂ solutions. <i>Molecular Physics</i> , 2001 , 99, 825-833	1.7	33
108	Parameterizing polarizable intermolecular potentials for water with the ice 1h phase. <i>Molecular Physics</i> , 1995 , 85, 81-90	1.7	32

107	Ferrous iron diffusion in ferro-periclase across the spin transition. <i>Earth and Planetary Science Letters</i> , 2011 , 302, 393-402	5.3	31
106	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
105	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
104	Anisotropy as cause for polarity reversals of D ₂ reflections. <i>Earth and Planetary Science Letters</i> , 2011 , 307, 369-376	5.3	30
103	The structure, ordering and equation of state of ammonia dihydrate (nh ₃ □2h ₂ o). <i>Icarus</i> , 2003 , 162, 59-73.8		29
102	The electrical conductivity and thermal profile of the Earth's mid-mantle. <i>Geophysical Research Letters</i> , 2000 , 27, 2325-2328	4.9	29
101	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
100	Theoretical investigation of metastable Al ₂ SiO ₅ polymorphs. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2001 , 57, 548-57		28
99	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
98	Seismic velocities of CaSiO perovskite can explain LLSVPs in Earth's lower mantle. <i>Nature</i> , 2019 , 572, 643-647	50.4	26
97	Structural and magnetic phase transitions in simple oxides using hybrid functionals. <i>Molecular Simulation</i> , 2005 , 31, 367-377	2	26
96	Zinc Complexation in Hydrothermal Chloride Brines: Results from ab Initio Molecular Dynamics Calculations. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 1050-1054	2.8	26
95	Dynamical properties of liquid water. <i>Journal of Physics Condensed Matter</i> , 1996 , 8, 9269-9274	1.8	25
94	Structural, vibrational and thermodynamic properties of Mg ₂ SiO ₄ and MgSiO ₃ minerals from first-principles simulations. <i>Physics of the Earth and Planetary Interiors</i> , 2015 , 240, 1-24	2.3	24
93	Dopant control over the crystal morphology of ceramic materials. <i>Surface Science</i> , 2007 , 601, 4793-4800.1.8		24
92	The effect of silicon impurities on the phase diagram of iron and possible implications for the Earth's core structure. <i>Journal of Physics and Chemistry of Solids</i> , 2008 , 69, 2177-2181	3.9	24
91	Ab initio simulation of the ice II structure. <i>Journal of Chemical Physics</i> , 2003 , 119, 4567-4572	3.9	24
90	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

89	Rheological control of Wadati-Benioff zone seismicity. <i>Geophysical Research Letters</i> , 1988 , 15, 1081-1084.	4.9	24
88	The Earth's core as a reservoir of water. <i>Nature Geoscience</i> , 2020 , 13, 453-458	18.3	23
87	Thermoelasticity of Fe ₇ C ₃ under inner core conditions. <i>Journal of Geophysical Research: Solid Earth</i> , 2016 , 121, 5828-5837	3.6	23
86	Seismic Anisotropy of Post-Perovskite and the Lowermost Mantle. <i>Geophysical Monograph Series</i> , 2007 , 171-189	1.1	23
85	The elastic properties of hcp-Fe 1-xSi x at Earth's inner-core conditions. <i>Earth and Planetary Science Letters</i> , 2016 , 451, 89-96	5.3	22
84	Melting properties from ab initio free energy calculations: Iron at the Earth's inner-core boundary. <i>Physical Review B</i> , 2018 , 98,	3.3	22
83	Shear-induced material transfer across the core-mantle boundary aided by the post-perovskite phase transition. <i>Earth, Planets and Space</i> , 2005 , 57, 459-464	2.9	21
82	Experimental verification of the Stokes-Einstein relation in liquid FeBeS at 5 GPa. <i>Molecular Physics</i> , 2001 , 99, 773-777	1.7	21
81	Ferrous iron partitioning in the lower mantle. <i>Physics of the Earth and Planetary Interiors</i> , 2016 , 257, 12-17.	3	21
80	Elastic properties of ferropericlase at lower mantle conditions and its relevance to ULVZs. <i>Earth and Planetary Science Letters</i> , 2015 , 417, 40-48	5.3	20
79	Equation of state of hexagonal closed packed iron under Earth's core conditions from quantum Monte Carlo calculations. <i>Physical Review B</i> , 2009 , 79,	3.3	20
78	Structure and elasticity of hydrous ringwoodite: A first principle investigation. <i>Physics of the Earth and Planetary Interiors</i> , 2009 , 177, 103-115	2.3	20
77	A convenient method for measuring ferric iron in magnesiowüstite (MgO-Fe _{1-x} O). <i>American Mineralogist</i> , 1998 , 83, 794-798	2.9	20
76	The use of a point polarizable dipole in intermolecular potentials for water. <i>Molecular Physics</i> , 1998 , 94, 873-876	1.7	20
75	Ab Initio Molecular Dynamics Investigation of Molten FeSiO in Earth's Core. <i>Geophysical Research Letters</i> , 2019 , 46, 6397-6405	4.9	19
74	Ab initio lattice dynamics calculations on the combined effect of temperature and silicon on the stability of different iron phases in the Earth's inner core. <i>Physics of the Earth and Planetary Interiors</i> , 2010 , 178, 2-7	2.3	19
73	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
72	Reconciling the Post-Perovskite Phase with Seismological Observations of Lowermost Mantle Structure. <i>Geophysical Monograph Series</i> , 2007 , 129-153	1.1	19

71	Elastic, thermal and structural properties of platinum. <i>Journal of Physics and Chemistry of Solids</i> , 2011 , 72, 169-175	3.9	18
70	An ab initio study of the compressional behavior of forsterite. <i>American Mineralogist</i> , 1996 , 81, 257-260	2.9	18
69	Water distribution in the lower mantle: Implications for hydrolytic weakening. <i>Earth and Planetary Science Letters</i> , 2018 , 484, 363-369	5.3	17
68	Simulating Diffusion. <i>Reviews in Mineralogy and Geochemistry</i> , 2010 , 71, 201-224	7.1	17
67	Phase transitions of BaCO ₃ at high pressures. <i>Mineralogical Magazine</i> , 2008 , 72, 659-665	1.7	17
66	Crystal morphology and surface structures of orthorhombic MgSiO ₃ perovskite. <i>Physics and Chemistry of Minerals</i> , 2005 , 31, 671-682	1.6	17
65	Molecular dynamics study of the dielectric constant of water under high pressure and temperature conditions. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1994 , 98, 906-911		16
64	Helium diffusion in olivine based on first principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2015 , 156, 145-153	5.5	15
63	Elastic properties of the post-perovskite phase of Fe ₂ O ₃ and implications for ultra-low velocity zones. <i>Physics of the Earth and Planetary Interiors</i> , 2008 , 170, 260-266	2.3	15
62	Lattice-Preferred Orientation of Lower Mantle Materials and Seismic Anisotropy in the D ₂ Layer. <i>Geophysical Monograph Series</i> , 2007 , 69-78	1.1	15
61	Ab initio simulations of iron-nickel alloys at Earth's core conditions. <i>Earth and Planetary Science Letters</i> , 2012 , 345-348, 126-130	5.3	14
60	Incorporation of Fe ³⁺ into forsterite and wadsleyite. <i>American Mineralogist</i> , 2000 , 85, 1155-1158	2.9	14
59	Relative strength of the pyrope-majorite solid solution and the flow-law of majorite containing garnets. <i>Physics of the Earth and Planetary Interiors</i> , 2010 , 179, 87-95	2.3	13
58	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
57	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
56	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
55	Carbon Partitioning Between the Earth's Inner and Outer Core. <i>Journal of Geophysical Research: Solid Earth</i> , 2019 , 124, 12812-12824	3.6	12
54	Elastic properties of ferrous bearing MgSiO ₃ and their relevance to ULVZs. <i>Geophysical Journal International</i> , 2015 , 201, 496-504	2.6	11

53	Diffusion of aluminium in MgO from first principles. <i>Physics and Chemistry of Minerals</i> , 2012 , 39, 503-514	1.6	11
52	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
51	Applications of Density Functional Theory in the Geosciences. <i>MRS Bulletin</i> , 2006 , 31, 675-680	3.2	11
50	The High-Temperature Elasticity of MgSiO ₃ Post-Perovskite. <i>Geophysical Monograph Series</i> , 2007 , 99-113	1.1	11
49	Collaborative grid infrastructure for molecular simulations: The eMinerals minigrid as a prototype integrated compute and data grid. <i>Molecular Simulation</i> , 2005 , 31, 303-313	2	11
48	Ab-initio simulations of magnetic iron sulphides. <i>Molecular Simulation</i> , 2005 , 31, 379-384	2	11
47	Self diffusion of argon in flexible, single wall, carbon nanotubes. <i>Molecular Simulation</i> , 2005 , 31, 385-389	2	11
46	The pressure medium as a solid-state oxygen buffer. <i>Geophysical Research Letters</i> , 1999 , 26, 259-262	4.9	11
45	The elastic properties and stability of fcc-Fe and fcc-FeNi alloys at inner-core conditions. <i>Geophysical Journal International</i> , 2015 , 202, 94-101	2.6	10
44	Stability and Reactions of CaCO ₃ Polymorphs in the Earth's Deep Mantle. <i>Journal of Geophysical Research: Solid Earth</i> , 2018 , 123, 6491	3.6	10
43	The isothermal equation of state of CaPtO ₃ post-perovskite to 40GPa. <i>Physics of the Earth and Planetary Interiors</i> , 2010 , 182, 113-118	2.3	10
42	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
41	Influence of the Post-Perovskite Transition on Thermal and Thermo-Chemical Mantle Convection. <i>Geophysical Monograph Series</i> , 2007 , 229-247	1.1	9
40	Elasticity of hydrous ringwoodite at mantle conditions: Implication for water distribution in the lowermost mantle transition zone. <i>Earth and Planetary Science Letters</i> , 2021 , 554, 116626	5.3	9
39	The phase diagrams of KCaF and NaMgF by ab initio simulations. <i>Physics and Chemistry of Minerals</i> , 2018 , 45, 311-322	1.6	8
38	Thermoelastic properties and crystal structure of CaPtO ₃ post-perovskite from 0 to 9 GPa and from 210 to 973 K. <i>Journal of Applied Crystallography</i> , 2011 , 44, 999-1016	3.8	8
37	Modeling the melting of multicomponent systems: the case of MgSiO ₃ perovskite under lower mantle conditions. <i>Scientific Reports</i> , 2016 , 6, 29830	4.9	8
36	Mg partitioning between solid and liquid iron under the Earth's core conditions. <i>Physics of the Earth and Planetary Interiors</i> , 2018 , 274, 218-221	2.3	7

35	Prospecting for water in the transition zone: $d \ln(V_s)/d \ln(V_p)$. <i>Physics of the Earth and Planetary Interiors</i> , 2011 , 189, 117-120	2.3	7
34	Structural phase transitions in IrO_2 at high pressures. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 045202	2.3	7
33	Discovery of Post-Perovskite Phase Transition and the Nature of D' Layer. <i>Geophysical Monograph Series</i> , 2007 , 19-35	1.1	7
32	Electronic Transitions and Spin States in the Lower Mantle. <i>Geophysical Monograph Series</i> , 2007 , 47-68	1.1	7
31	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
30	Deformation of olivine at 5GPa and 3500°C. <i>Physics of the Earth and Planetary Interiors</i> , 2009 , 172, 84-90	2.3	6
29	Strong shear softening induced by superionic hydrogen in Earth's inner core. <i>Earth and Planetary Science Letters</i> , 2021 , 568, 117014	5.3	6
28	Grain-boundary enrichment of iron on magnesium silicate perovskite. <i>European Journal of Mineralogy</i> , 2007 , 19, 617-622	2.2	5
27	Constraints on the Presence or Absence of Post-Perovskite in the Lowermost Mantle from Long-Period Seismology. <i>Geophysical Monograph Series</i> , 2007 , 191-216	1.1	5
26	The Dynamical Influences from Physical Properties in the Lower Mantle and Post-Perovskite Phase Transition. <i>Geophysical Monograph Series</i> , 2007 , 249-270	1.1	5
25	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
24	. <i>Geophysical Monograph Series</i> , 2007 ,	1.1	4
23	Anisotropic diffusion creep in postperovskite provides a new model for deformation at the core-mantle boundary. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 ,	11.5	4
22	High-pressure silica phase transitions: Implications for deep mantle dynamics and silica crystallization in the protocore. <i>American Mineralogist</i> , 2020 , 105, 1014-1020	2.9	3
21	Deformation-Induced Mechanical Instabilities at the Core-Mantle Boundary. <i>Geophysical Monograph Series</i> , 2007 , 271-287	1.1	3
20	A computational study of the effect of Li^+ solid solutions on the structures and stabilities of layered silicate materials—An application of the use of Condor pools in molecular simulation. <i>Molecular Simulation</i> , 2005 , 31, 339-347	2	3
19	Sulfur isotopic signature of Earth established by planetesimal volatile evaporation. <i>Nature Geoscience</i> ,	18.3	3
18	Equation of State of hcp Fe-C-Si Alloys and the Effect of C Incorporation Mechanism on the Density of hcp Fe Alloys at 300K. <i>Journal of Geophysical Research: Solid Earth</i> , 2020 , 125, e2020JB020159	3.6	2

17	10. Simulating Diffusion 2010 , 201-224		2
16	An Introduction to Post-Perovskite: The Last Mantle Phase Transition. <i>Geophysical Monograph Series</i> , 2007 , 1-7	1.1	2
15	Effect of Iron on the Properties of Post-Perovskite Silicate. <i>Geophysical Monograph Series</i> , 2007 , 37-46	1.1	2
14	The effect of water on the post-spinel transition and evidence for extreme water contents at the bottom of the transition zone. <i>Earth and Planetary Science Letters</i> , 2021 , 565, 116909	5.3	2
13	Ferric iron in bridgmanite and implications for ULVZs. <i>Physics of the Earth and Planetary Interiors</i> , 2020 , 306, 106505	2.3	1
12	Habitable Planets: Interior Dynamics and Long-Term Evolution. <i>Proceedings of the International Astronomical Union</i> , 2012 , 8, 339-349	0.1	1
11	Thermodynamic Properties and Stability Field of MgSiO ₃ Post-Perovskite. <i>Geophysical Monograph Series</i> , 2007 , 79-97	1.1	1
10	The coupled effects of mantle mixing and a water-dependent viscosity on the surface ocean. <i>Earth and Planetary Science Letters</i> , 2020 , 530, 115881	5.3	1
9	The discontinuous effect of pressure on twin boundary strength in MgO. <i>Physics and Chemistry of Minerals</i> , 2020 , 47, 1	1.6	0
8	ElaT: A toolkit for thermoelastic calculations. <i>Computer Physics Communications</i> , 2022 , 273, 108280	4.2	0
7	Hydrous silicate melts and the deep mantle H ₂ O cycle. <i>Earth and Planetary Science Letters</i> , 2022 , 581, 117408	5.3	0
6	Diffusion of noble gases in subduction zone hydrous minerals. <i>Geochimica Et Cosmochimica Acta</i> , 2020 , 291, 50-61	5.5	0
5	Structural evolution in a pyrolitic magma ocean under mantle conditions. <i>Earth and Planetary Science Letters</i> , 2022 , 584, 117473	5.3	0
4	Reply to the comment by Z. Duan, N. Mørner, and J. H. Weare on Measurement of the PVT properties of water to 25 kbars and 1600°C from synthetic fluid inclusions in corundum. <i>Geochimica Et Cosmochimica Acta</i> , 1995 , 59, 2641	5.5	
3	Incorporation of tetrahedral ferric iron into hydrous ringwoodite. <i>American Mineralogist</i> , 2021 , 106, 900-908		0
2	Equation of state for CO and CO ₂ fluids and their application on decarbonation reactions at high pressure and temperature. <i>Chemical Geology</i> , 2021 , 559, 119918	4.2	
1	Nitrogen Speciation in Silicate Melts at Mantle Conditions From Ab Initio Simulations. <i>Geophysical Research Letters</i> , 2022 , 49,	4.9	