

# J P Brodholt

## 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.

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	ElaT: A toolkit for thermoelastic calculations. <i>Computer Physics Communications</i> , <b>2022</b> , 273, 108280	4.2	0
177	Hydrous silicate melts and the deep mantle H <sub>2</sub> O cycle. <i>Earth and Planetary Science Letters</i> , <b>2022</b> , 581, 117408	5.3	0
176	Nitrogen Speciation in Silicate Melts at Mantle Conditions From Ab Initio Simulations. <i>Geophysical Research Letters</i> , <b>2022</b> , 49,	4.9	
175	Structural evolution in a pyrolitic magma ocean under mantle conditions. <i>Earth and Planetary Science Letters</i> , <b>2022</b> , 584, 117473	5.3	0
174	Incorporation of tetrahedral ferric iron into hydrous ringwoodite. <i>American Mineralogist</i> , <b>2021</b> , 106, 900-908		
173	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> , <b>2021</b> , 565, 116909	5.3	2
172	Equation of state for CO and CO <sub>2</sub> fluids and their application on decarbonation reactions at high pressure and temperature. <i>Chemical Geology</i> , <b>2021</b> , 559, 119918	4.2	
171	Elasticity of hydrous ringwoodite at mantle conditions: Implication for water distribution in the lowermost mantle transition zone. <i>Earth and Planetary Science Letters</i> , <b>2021</b> , 554, 116626	5.3	9
170	Strong shear softening induced by superionic hydrogen in Earth's inner core. <i>Earth and Planetary Science Letters</i> , <b>2021</b> , 568, 117014	5.3	6
169	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> , <b>2020</b> , 125, e2020JB020159	3.6	2
168	The Earth's core as a reservoir of water. <i>Nature Geoscience</i> , <b>2020</b> , 13, 453-458	18.3	23
167	Ferric iron in bridgmanite and implications for ULVZs. <i>Physics of the Earth and Planetary Interiors</i> , <b>2020</b> , 306, 106505	2.3	1
166	The discontinuous effect of pressure on twin boundary strength in MgO. <i>Physics and Chemistry of Minerals</i> , <b>2020</b> , 47, 1	1.6	0
165	High-pressure silica phase transitions: Implications for deep mantle dynamics and silica crystallization in the protocore. <i>American Mineralogist</i> , <b>2020</b> , 105, 1014-1020	2.9	3
164	The coupled effects of mantle mixing and a water-dependent viscosity on the surface ocean. <i>Earth and Planetary Science Letters</i> , <b>2020</b> , 530, 115881	5.3	1
163	Diffusion of noble gases in subduction zone hydrous minerals. <i>Geochimica Et Cosmochimica Acta</i> , <b>2020</b> , 291, 50-61	5.5	0
162	Ab Initio Molecular Dynamics Investigation of Molten Fe <sub>3</sub> Si in Earth's Core. <i>Geophysical Research Letters</i> , <b>2019</b> , 46, 6397-6405	4.9	19

161	Seismic velocities of CaSiO perovskite can explain LLSVPs in Earth's lower mantle. <i>Nature</i> , <b>2019</b> , 572, 643-647	50.4	26
160	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> , <b>2019</b> ,	11.5	4
159	Carbon Partitioning Between the Earth's Inner and Outer Core. <i>Journal of Geophysical Research: Solid Earth</i> , <b>2019</b> , 124, 12812-12824	3.6	12
158	Water distribution in the lower mantle: Implications for hydrolytic weakening. <i>Earth and Planetary Science Letters</i> , <b>2018</b> , 484, 363-369	5.3	17
157	Mg partitioning between solid and liquid iron under the Earth's core conditions. <i>Physics of the Earth and Planetary Interiors</i> , <b>2018</b> , 274, 218-221	2.3	7
156	The phase diagrams of KCaF and NaMgF by ab initio simulations. <i>Physics and Chemistry of Minerals</i> , <b>2018</b> , 45, 311-322	1.6	8
155	Stability and Reactions of CaCO <sub>3</sub> Polymorphs in the Earth's Deep Mantle. <i>Journal of Geophysical Research: Solid Earth</i> , <b>2018</b> , 123, 6491	3.6	10
154	The elastic properties of hcp-Fe alloys under the conditions of the Earth's inner core. <i>Earth and Planetary Science Letters</i> , <b>2018</b> , 493, 118-127	5.3	38
153	Melting properties from ab initio free energy calculations: Iron at the Earth's inner-core boundary. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	22
152	Composition of the low seismic velocity E' layer at the top of Earth's core. <i>Geophysical Research Letters</i> , <b>2017</b> , 44, 8303-8310	4.9	39
151	Thermoelasticity of Fe <sub>7</sub> C <sub>3</sub> under inner core conditions. <i>Journal of Geophysical Research: Solid Earth</i> , <b>2016</b> , 121, 5828-5837	3.6	23
150	Modeling the melting of multicomponent systems: the case of MgSiO <sub>3</sub> perovskite under lower mantle conditions. <i>Scientific Reports</i> , <b>2016</b> , 6, 29830	4.9	8
149	The elastic properties of hcp-Fe 1-x Si x at Earth's inner-core conditions. <i>Earth and Planetary Science Letters</i> , <b>2016</b> , 451, 89-96	5.3	22
148	Ferrous iron partitioning in the lower mantle. <i>Physics of the Earth and Planetary Interiors</i> , <b>2016</b> , 257, 12-17.3	17.3	21
147	Elastic properties of ferropericlase at lower mantle conditions and its relevance to ULVZs. <i>Earth and Planetary Science Letters</i> , <b>2015</b> , 417, 40-48	5.3	20
146	Elastic properties of ferrous bearing MgSiO <sub>3</sub> and their relevance to ULVZs. <i>Geophysical Journal International</i> , <b>2015</b> , 201, 496-504	2.6	11
145	The elastic properties and stability of fcc-Fe and fcc-FeNi alloys at inner-core conditions. <i>Geophysical Journal International</i> , <b>2015</b> , 202, 94-101	2.6	10
144	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> , <b>2015</b> , 112, 12310-4	11.5	94

143	Structural, vibrational and thermodynamic properties of Mg <sub>2</sub> SiO <sub>4</sub> and MgSiO <sub>3</sub> minerals from first-principles simulations. <i>Physics of the Earth and Planetary Interiors</i> , <b>2015</b> , 240, 1-24	2.3	24
142	Helium diffusion in olivine based on first principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , <b>2015</b> , 156, 145-153	5.5	15
141	Variation of thermal conductivity and heat flux at the Earth's core mantle boundary. <i>Earth and Planetary Science Letters</i> , <b>2014</b> , 390, 175-185	5.3	37
140	A seismologically consistent compositional model of Earth's core. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2014</b> , 111, 7542-5	11.5	167
139	Mantle dynamics in super-Earths: Post-perovskite rheology and self-regulation of viscosity. <i>Icarus</i> , <b>2013</b> , 225, 50-61	3.8	101
138	Elastic properties of MgSiO <sub>3</sub> -perovskite under lower mantle conditions and the composition of the deep Earth. <i>Earth and Planetary Science Letters</i> , <b>2013</b> , 379, 1-12	5.3	50
137	Strong premelting effect in the elastic properties of hcp-Fe under inner-core conditions. <i>Science</i> , <b>2013</b> , 342, 466-8	33.3	81
136	The incorporation of water into lower-mantle perovskites: A first-principles study. <i>Earth and Planetary Science Letters</i> , <b>2013</b> , 364, 37-43	5.3	36
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> , <b>2013</b> , 365, 143-151	5.3	47
134	Ab initio simulations of iron-nickel alloys at Earth's core conditions. <i>Earth and Planetary Science Letters</i> , <b>2012</b> , 345-348, 126-130	5.3	14
133	Diffusion of aluminium in MgO from first principles. <i>Physics and Chemistry of Minerals</i> , <b>2012</b> , 39, 503-514	1.6	11
132	Habitable Planets: Interior Dynamics and Long-Term Evolution. <i>Proceedings of the International Astronomical Union</i> , <b>2012</b> , 8, 339-349	0.1	1
131	Ferrous iron diffusion in ferro-periclase across the spin transition. <i>Earth and Planetary Science Letters</i> , <b>2011</b> , 302, 393-402	5.3	31
130	Anisotropy as cause for polarity reversals of D <sub>2</sub> reflections. <i>Earth and Planetary Science Letters</i> , <b>2011</b> , 307, 369-376	5.3	30
129	Prospecting for water in the transition zone: d ln(V <sub>s</sub> )/d ln(V <sub>p</sub> ). <i>Physics of the Earth and Planetary Interiors</i> , <b>2011</b> , 189, 117-120	2.3	7
128	Ab initio molecular dynamic simulation on the elasticity of Mg <sub>3</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> pyrope. <i>Journal of Earth Science (Wuhan, China)</i> , <b>2011</b> , 22, 169-175	2.2	11
127	Thermoelastic properties and crystal structure of CaPtO <sub>3</sub> post-perovskite from 0 to 9 GPa and from 200 to 973 K. <i>Journal of Applied Crystallography</i> , <b>2011</b> , 44, 999-1016	3.8	8
126	Elastic, thermal and structural properties of platinum. <i>Journal of Physics and Chemistry of Solids</i> , <b>2011</b> , 72, 169-175	3.9	18

125	First-principles constraints on diffusion in lower-mantle minerals and a weak D'' layer. <i>Nature</i> , <b>2010</b> , 465, 462-5	50.4	181
124	10. Simulating Diffusion <b>2010</b> , 201-224		2
123	Simulating Diffusion. <i>Reviews in Mineralogy and Geochemistry</i> , <b>2010</b> , 71, 201-224	7.1	17
122	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> , <b>2010</b> , 178, 2-7	2.3	19
121	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> , <b>2010</b> , 179, 87-95	2.3	13
120	The isothermal equation of state of CaPtO <sub>3</sub> post-perovskite to 40GPa. <i>Physics of the Earth and Planetary Interiors</i> , <b>2010</b> , 182, 113-118	2.3	10
119	DFT study of migration enthalpies in MgSiO <sub>3</sub> perovskite. <i>Physics and Chemistry of Minerals</i> , <b>2009</b> , 36, 151-158	1.6	38
118	Weakening of calcium iridate during its transformation from perovskite to post-perovskite. <i>Nature Geoscience</i> , <b>2009</b> , 2, 794-797	18.3	66
117	Equation of state of hexagonal closed packed iron under Earth's core conditions from quantum Monte Carlo calculations. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	20
116	Deformation of olivine at 5GPa and 3500°C. <i>Physics of the Earth and Planetary Interiors</i> , <b>2009</b> , 172, 84-90	2.3	6
115	Ab initio molecular dynamics study of elasticity of akimotoite MgSiO <sub>3</sub> at mantle conditions. <i>Physics of the Earth and Planetary Interiors</i> , <b>2009</b> , 173, 115-120	2.3	12
114	Structure and elasticity of hydrous ringwoodite: A first principle investigation. <i>Physics of the Earth and Planetary Interiors</i> , <b>2009</b> , 177, 103-115	2.3	20
113	Light elements in the core: Effects of impurities on the phase diagram of iron. <i>Geophysical Research Letters</i> , <b>2008</b> , 35,	4.9	33
112	Elastic properties of the post-perovskite phase of Fe <sub>2</sub> O <sub>3</sub> and implications for ultra-low velocity zones. <i>Physics of the Earth and Planetary Interiors</i> , <b>2008</b> , 170, 260-266	2.3	15
111	The stability of bcc-Fe at high pressures and temperatures with respect to tetragonal strain. <i>Physics of the Earth and Planetary Interiors</i> , <b>2008</b> , 170, 52-59	2.3	31
110	High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores. <i>Earth and Planetary Science Letters</i> , <b>2008</b> , 272, 481-487	5.3	46
109	Ab initio molecular dynamics simulations for thermal equation of state of B2-type NaCl. <i>Journal of Applied Physics</i> , <b>2008</b> , 103, 023510	2.5	19
108	Phase transitions of BaCO <sub>3</sub> at high pressures. <i>Mineralogical Magazine</i> , <b>2008</b> , 72, 659-665	1.7	17

107	Structural phase transitions in IrO <sub>2</sub> at high pressures. <i>Journal of Physics Condensed Matter</i> , <b>2008</b> , 20, 045202	202	7
106	The long-term stability of a possible aqueous ammonium sulfate ocean inside Titan. <i>Icarus</i> , <b>2008</b> , 197, 137-151	3.8	66
105	First-principles simulation of high-pressure polymorphs in MgAl <sub>2</sub> O <sub>4</sub> . <i>Physics and Chemistry of Minerals</i> , <b>2008</b> , 35, 381-386	1.6	28
104	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> , <b>2008</b> , 69, 2177-2181	3.9	24
103	An Introduction to Post-Perovskite: The Last Mantle Phase Transition. <i>Geophysical Monograph Series</i> , <b>2007</b> , 1-7	1.1	2
102	Discovery of Post-Perovskite Phase Transition and the Nature of D' Layer. <i>Geophysical Monograph Series</i> , <b>2007</b> , 19-35	1.1	7
101	Dopant control over the crystal morphology of ceramic materials. <i>Surface Science</i> , <b>2007</b> , 601, 4793-4800	1.8	24
100	Grain-boundary enrichment of iron on magnesium silicate perovskite. <i>European Journal of Mineralogy</i> , <b>2007</b> , 19, 617-622	2.2	5
99	Electronic spin transitions in iron-bearing MgSiO <sub>3</sub> perovskite. <i>Earth and Planetary Science Letters</i> , <b>2007</b> , 253, 282-290	5.3	89
98	The effect of cation-ordering on the elastic properties of majorite: An ab initio study. <i>Earth and Planetary Science Letters</i> , <b>2007</b> , 256, 28-35	5.3	12
97	Chemical versus thermal heterogeneity in the lower mantle: The most likely role of anelasticity. <i>Earth and Planetary Science Letters</i> , <b>2007</b> , 262, 429-437	5.3	41
96	Arsenic incorporation into FeS <sub>2</sub> pyrite and its influence on dissolution: A DFT study. <i>Geochimica Et Cosmochimica Acta</i> , <b>2007</b> , 71, 624-630	5.5	117
95	Effect of Iron on the Properties of Post-Perovskite Silicate. <i>Geophysical Monograph Series</i> , <b>2007</b> , 37-46	1.1	2
94	Electronic Transitions and Spin States in the Lower Mantle. <i>Geophysical Monograph Series</i> , <b>2007</b> , 47-68	1.1	7
93	Lattice-Preferred Orientation of Lower Mantle Materials and Seismic Anisotropy in the D' Layer. <i>Geophysical Monograph Series</i> , <b>2007</b> , 69-78	1.1	15
92	Thermodynamic Properties and Stability Field of MgSiO <sub>3</sub> Post-Perovskite. <i>Geophysical Monograph Series</i> , <b>2007</b> , 79-97	1.1	1
91	The High-Temperature Elasticity of MgSiO <sub>3</sub> Post-Perovskite. <i>Geophysical Monograph Series</i> , <b>2007</b> , 99-113	1.1	11
90	Reconciling the Post-Perovskite Phase with Seismological Observations of Lowermost Mantle Structure. <i>Geophysical Monograph Series</i> , <b>2007</b> , 129-153	1.1	19

89	Seismic Anisotropy of Post-Perovskite and the Lowermost Mantle. <i>Geophysical Monograph Series</i> , <b>2007</b> , 171-189	1.1	23
88	Constraints on the Presence or Absence of Post-Perovskite in the Lowermost Mantle from Long-Period Seismology. <i>Geophysical Monograph Series</i> , <b>2007</b> , 191-216	1.1	5
87	Influence of the Post-Perovskite Transition on Thermal and Thermo-Chemical Mantle Convection. <i>Geophysical Monograph Series</i> , <b>2007</b> , 229-247	1.1	9
86	The Dynamical Influences from Physical Properties in the Lower Mantle and Post-Perovskite Phase Transition. <i>Geophysical Monograph Series</i> , <b>2007</b> , 249-270	1.1	5
85	Deformation-Induced Mechanical Instabilities at the Core-Mantle Boundary. <i>Geophysical Monograph Series</i> , <b>2007</b> , 271-287	1.1	3
84	. <i>Geophysical Monograph Series</i> , <b>2007</b> ,	1.1	4
83	Applications of Density Functional Theory in the Geosciences. <i>MRS Bulletin</i> , <b>2006</b> , 31, 675-680	3.2	11
82	Elastic anisotropy of FeSiO <sub>3</sub> end-members of the perovskite and post-perovskite phases. <i>Geophysical Research Letters</i> , <b>2006</b> , 33, n/a-n/a	4.9	55
81	Ab initio study of the phase separation of argon in molten iron at high pressures. <i>Geophysical Research Letters</i> , <b>2006</b> , 33,	4.9	7
80	Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO <sub>3</sub> post-perovskite. <i>Geophysical Research Letters</i> , <b>2006</b> , 33,	4.9	44
79	Unsolved problems in the lowermost mantle. <i>Geophysical Research Letters</i> , <b>2006</b> , 33,	4.9	33
78	First-principles modelling of Earth and planetary materials at high pressures and temperatures. <i>Reports on Progress in Physics</i> , <b>2006</b> , 69, 2365-2441	14.4	133
77	Elasticity of CaSiO <sub>3</sub> perovskite at high pressure and high temperature. <i>Physics of the Earth and Planetary Interiors</i> , <b>2006</b> , 155, 249-259	2.3	72
76	Phase stability of CaSiO <sub>3</sub> perovskite at high pressure and temperature: Insights from ab initio molecular dynamics. <i>Physics of the Earth and Planetary Interiors</i> , <b>2006</b> , 155, 260-268	2.3	40
75	Elasticity of Mg <sub>2</sub> SiO <sub>4</sub> ringwoodite at mantle conditions. <i>Physics of the Earth and Planetary Interiors</i> , <b>2006</b> , 157, 181-187	2.3	27
74	Collaborative grid infrastructure for molecular simulations: The eMinerals minigrid as a prototype integrated compute and data grid. <i>Molecular Simulation</i> , <b>2005</b> , 31, 303-313	2	11
73	Structural and magnetic phase transitions in simple oxides using hybrid functionals. <i>Molecular Simulation</i> , <b>2005</b> , 31, 367-377	2	26
72	Ab-initio simulations of magnetic iron sulphides. <i>Molecular Simulation</i> , <b>2005</b> , 31, 379-384	2	11



71	Quantum Monte Carlo calculations of the structural properties and the B1-B2 phase transition of MgO. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	53
70	Shear-induced material transfer across the core-mantle boundary aided by the post-perovskite phase transition. <i>Earth, Planets and Space</i> , <b>2005</b> , 57, 459-464	2.9	21
69	Self diffusion of argon in flexible, single wall, carbon nanotubes. <i>Molecular Simulation</i> , <b>2005</b> , 31, 385-389		11
68	The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO <sub>3</sub> . <i>Earth and Planetary Science Letters</i> , <b>2005</b> , 230, 1-10	5.3	129
67	Elasticity of (Mg, Fe)(Si, Al)O <sub>3</sub> -perovskite at high pressure. <i>Earth and Planetary Science Letters</i> , <b>2005</b> , 240, 529-536	5.3	38
66	CaSiO <sub>3</sub> perovskite at lower mantle pressures. <i>Geophysical Research Letters</i> , <b>2005</b> , 32,	4.9	42
65	Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. <i>Geophysical Research Letters</i> , <b>2005</b> , 32,	4.9	42
64	High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al <sub>2</sub> O <sub>3</sub> . <i>Geophysical Research Letters</i> , <b>2005</b> , 32,	4.9	35
63	Electronic structure study of the high-pressure vibrational spectrum of FeS <sub>2</sub> pyrite. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 22067-73	3.4	31
62	Two-electron dissociation of single molecules by atomic manipulation at room temperature. <i>Nature</i> , <b>2005</b> , 434, 367-71	50.4	161
61	Subducted banded iron formations as a source of ultralow-velocity zones at the core-mantle boundary. <i>Nature</i> , <b>2005</b> , 434, 371-4	50.4	124
60	Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. <i>Nature</i> , <b>2005</b> , 438, 1004-7	50.4	175
59	Crystal morphology and surface structures of orthorhombic MgSiO <sub>3</sub> perovskite. <i>Physics and Chemistry of Minerals</i> , <b>2005</b> , 31, 671-682	1.6	17
58	Crystal morphology and surface structures of orthorhombic MgSiO <sub>3</sub> in the presence of divalent impurity ions. <i>Physics and Chemistry of Minerals</i> , <b>2005</b> , 32, 379-387	1.6	5
57	A computational study of the effect of Li <sup>+</sup> 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> , <b>2005</b> , 31, 339-347	2	3
56	Electronic structure of the antiferromagnetic B1-structured FeO. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	53
55	The influence of potassium on core and geodynamo evolution. <i>Geophysical Journal International</i> , <b>2004</b> , 156, 363-376	2.6	152
54	Thermal expansion and crystal structure of cementite, Fe <sub>3</sub> C, between 4 and 600 K determined by time-of-flight neutron powder diffraction. <i>Journal of Applied Crystallography</i> , <b>2004</b> , 37, 82-90	3.8	153



53	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> , <b>2004</b> , 222, 501-516	5.3	65
52	The structure, ordering and equation of state of ammonia dihydrate (NH <sub>3</sub> · 2H <sub>2</sub> O). <i>Icarus</i> , <b>2003</b> , 162, 59-73.8		29
51	Possible thermal and chemical stabilization of body-centred-cubic iron in the Earth's core. <i>Nature</i> , <b>2003</b> , 424, 536-9	50.4	219
50	Ab initio simulation of the ice II structure. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 4567-4572	3.9	24
49	Zinc Complexation in Hydrothermal Chloride Brines: Results from ab Initio Molecular Dynamics Calculations. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 1050-1054	2.8	26
48	Hydration of Sr <sup>2+</sup> in Hydrothermal Solutions from ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2003</b> , 107, 9056-9058	3.4	35
47	Hydrogen bonding in solid ammonia from ab initio calculations. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 5987-5994	3.9	44
46	A high-resolution neutron powder diffraction study of ammonia dihydrate (NH <sub>3</sub> · 2H <sub>2</sub> O) phase I. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 10806-10813	3.9	33
45	Computational mineral physics and the physical properties of perovskite. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , <b>2002</b> , 360, 2507-20	3	13
44	The ab initio simulation of the Earth's core. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , <b>2002</b> , 360, 1227-44	3	24
43	The effect of ferromagnetism on the equation of state of Fe <sub>3</sub> C studied by first-principles calculations. <i>Earth and Planetary Science Letters</i> , <b>2002</b> , 203, 567-575	5.3	102
42	Experimental verification of the Stokes-Einstein relation in liquid Fe <sub>7</sub> FeS at 5 GPa. <i>Molecular Physics</i> , <b>2001</b> , 99, 773-777	1.7	21
41	Theoretical investigation of metastable Al <sub>2</sub> SiO <sub>5</sub> polymorphs. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2001</b> , 57, 548-57		28
40	The elastic constants of MgSiO <sub>3</sub> perovskite at pressures and temperatures of the Earth's mantle. <i>Nature</i> , <b>2001</b> , 411, 934-7	50.4	172
39	Molecular Dynamics simulation of aqueous ZnCl <sub>2</sub> solutions. <i>Molecular Physics</i> , <b>2001</b> , 99, 825-833	1.7	33
38	Ab initio simulation of ammonia monohydrate (NH <sub>3</sub> · H <sub>2</sub> O) and ammonium hydroxide (NH <sub>4</sub> OH). <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 7006-7014	3.9	41
37	Ab initio elasticity and thermal equation of state of MgSiO <sub>3</sub> perovskite. <i>Earth and Planetary Science Letters</i> , <b>2001</b> , 184, 555-560	5.3	125
36	Incorporation of Fe <sup>3+</sup> into forsterite and wadsleyite. <i>American Mineralogist</i> , <b>2000</b> , 85, 1155-1158	2.9	14

35	In situ measurement of viscosity of liquids in the Fe-FeS system at high pressures and temperatures. <i>American Mineralogist</i> , <b>2000</b> , 85, 1838-1842	2.9	81
34	Pressure-induced changes in the compression mechanism of aluminous perovskite in the Earth's mantle. <i>Nature</i> , <b>2000</b> , 407, 620-2	50.4	124
33	High-pressure phases in the Al <sub>2</sub> SiO <sub>5</sub> system and the problem of aluminous phase in the Earth's lower mantle: ab initio calculations. <i>Physics and Chemistry of Minerals</i> , <b>2000</b> , 27, 430-439	1.6	45
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29	An ab initio study of hydrogen in forsterite and a possible mechanism for hydrolytic weakening. <i>Journal of Geophysical Research</i> , <b>2000</b> , 105, 18977-18982		65
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24	Molecular dynamics simulations of aqueous NaCl solutions at high pressures and temperatures. <i>Chemical Geology</i> , <b>1998</b> , 151, 11-19	4.2	85
23	Analysis of the hydrogen-bonded structure of water from ambient to supercritical conditions. <i>Journal of Chemical Physics</i> , <b>1998</b> , 108, 8528-8540	3.9	165
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15	Dynamical properties of liquid water. <i>Journal of Physics Condensed Matter</i> , <b>1996</b> , 8, 9269-9274	1.8	25
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