## Lars P Stixrude

## List of Publications by Citations

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8,619 133 51 91 h-index g-index citations papers 8.1 6.35 142 9,314 L-index avg, IF ext. citations ext. papers

#	Paper	IF	Citations
133	Thermodynamics of mantle minerals - I. Physical properties. <i>Geophysical Journal International</i> , <b>2005</b> , 162, 610-632	2.6	405
132	Thermodynamics of mantle minerals - II. Phase equilibria. <i>Geophysical Journal International</i> , <b>2011</b> , 184, 1180-1213	2.6	376
131	Structure and elasticity of MgO at high pressure. <i>American Mineralogist</i> , <b>1997</b> , 82, 51-60	2.9	372
130	First-principles elastic constants for the hcp transition metals Fe, Co, and Re at high pressure. <i>Physical Review B</i> , <b>1999</b> , 60, 791-799	3.3	325
129	Petrology, elasticity, and composition of the mantle transition zone. <i>Journal of Geophysical Research</i> , <b>1992</b> , 97, 6849		324
128	The effect of bulk composition and temperature on mantle seismic structure. <i>Earth and Planetary Science Letters</i> , <b>2008</b> , 275, 70-79	5.3	273
127	Structure and freezing of MgSiO3 liquid in Earthß lower mantle. <i>Science</i> , <b>2005</b> , 310, 297-9	33.3	243
126	High-Pressure Elasticity of Iron and Anisotropy of Earth Is Inner Core. Science, 1995, 267, 1972-5	33.3	228
125	Elasticity of iron at the temperature of the Earthß inner core. <i>Nature</i> , <b>2001</b> , 413, 57-60	50.4	220
124	Mineralogy and elasticity of the oceanic upper mantle: Origin of the low-velocity zone. <i>Journal of Geophysical Research</i> , <b>2005</b> , 110,		212
123	Iron at high pressure: Linearized-augmented-plane-wave computations in the generalized-gradient approximation. <i>Physical Review B</i> , <b>1994</b> , 50, 6442-6445	3.3	206
122	High-pressure elastic properties of major materials of Earthß mantle from first principles. <i>Reviews of Geophysics</i> , <b>2001</b> , 39, 507-534	23.1	199
121	Thermodynamics of silicate liquids in the deep Earth. Earth and Planetary Science Letters, 2009, 278, 226	5- <del>3</del> .32	165
120	Thermoelasticity of Silicate Perovskite and Magnesiowustite and Stratification of the Earthß Mantle. <i>Science</i> , <b>1992</b> , 257, 1099-101	33.3	153
119	Thermal properties of iron at high pressures and temperatures. <i>Physical Review B</i> , <b>1996</b> , 53, 8296-8309	3.3	146
118	Ab initio studies of high-pressure structural transformations in silica. <i>Physical Review B</i> , <b>1997</b> , 55, 3465-	 3 <del>4</del> .731	131
117	First-principles simulations of liquid silica: Structural and dynamical behavior at high pressure. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	128

## (2002-1997)

116	Elastic properties of orthorhombic MgSiO3perovskite at lower mantle pressures. <i>American Mineralogist</i> , <b>1997</b> , 82, 635-638	2.9	124
115	First-principles calculation of defect-formation energies in the Y2(Ti,Sn,Zr)2O7 pyrochlore. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	123
114	Structure and sharpness of phase transitions and mantle discontinuities. <i>Journal of Geophysical Research</i> , <b>1997</b> , 102, 14835-14852		120
113	Self-consistent thermodynamic description of silicate liquids, with application to shock melting of MgO periclase and MgSiO3perovskite. <i>Geophysical Journal International</i> , <b>2009</b> , 178, 162-179	2.6	118
112	Ab initio elasticity of three high-pressure polymorphs of silica. <i>Geophysical Research Letters</i> , <b>1997</b> , 24, 3269-3272	4.9	115
111	Composition and temperature of Earth® inner core. <i>Journal of Geophysical Research</i> , <b>1997</b> , 102, 24729-2	4739	112
110	Hydrous silicate melt at high pressure. <i>Nature</i> , <b>2008</b> , 452, 983-6	50.4	112
109	Thermodynamics, structure, dynamics, and freezing of Mg2SiO4 liquid at high pressure. <i>Geochimica Et Cosmochimica Acta</i> , <b>2008</b> , 72, 1427-1441	5.5	110
108	Geophysics of Chemical Heterogeneity in the Mantle. <i>Annual Review of Earth and Planetary Sciences</i> , <b>2012</b> , 40, 569-595	15.3	109
107	Stability of orthorhombic MgSiO3 perovskite in the Earthß lower mantle. <i>Nature</i> , <b>1993</b> , 364, 613-616	50.4	108
106	Influence of phase transformations on lateral heterogeneity and dynamics in Earth® mantle. <i>Earth and Planetary Science Letters</i> , <b>2007</b> , 263, 45-55	5.3	107
105	Thermal conductivity of periclase (MgO) from first principles. <i>Physical Review Letters</i> , <b>2010</b> , 104, 208501	7.4	101
104	Viscosity of MgSiO3 liquid at Earth® mantle conditions: implications for an early magma ocean. <i>Science</i> , <b>2010</b> , 328, 740-2	33.3	97
103	Fundamental thermodynamic relations and silicate melting with implications for the constitution of D?. <i>Journal of Geophysical Research</i> , <b>1990</b> , 95, 19311		97
102	The 10[phase: a high-pressure expandable sheet silicate stable during subduction of hydrated lithosphere. <i>Earth and Planetary Science Letters</i> , <b>2001</b> , 186, 125-141	5.3	90
101	Tight-binding computations of elastic anisotropy of Fe, Xe, and Si under compression. <i>Physical Review B</i> , <b>1997</b> , 56, 8575-8589	3.3	89
100	EChO. Experimental Astronomy, 2012, 34, 311-353	1.3	82
99	First-principles study of illite-smectite and implications for clay mineral systems. <i>Nature</i> , <b>2002</b> , 420, 165-	<b>-8</b> 0.4	78

98	Elasticity of (Mg,Fe)SiO3-perovskite at high pressures. <i>Geophysical Research Letters</i> , <b>2002</b> , 29, 34-1	4.9	78
97	Magnetism in dense hexagonal iron. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2004</b> , 101, 33-6	11.5	76
96	Structure and elasticity of serpentine at high-pressure. <i>Earth and Planetary Science Letters</i> , <b>2009</b> , 279, 11-19	5.3	75
95	Correlation of seismic and petrologic thermometers suggests deep thermal anomalies beneath hotspots. <i>Earth and Planetary Science Letters</i> , <b>2007</b> , 264, 308-316	5.3	73
94	Hydrogen incorporation in stishovite at high pressure and symmetric hydrogen bonding in EALOOH. <i>Earth and Planetary Science Letters</i> , <b>2004</b> , 221, 421-431	5.3	73
93	Thermodynamics of the MgOBiO2 liquid system in Earthß lowermost mantle from first principles. <i>Earth and Planetary Science Letters</i> , <b>2013</b> , 361, 58-63	5.3	70
92	Structure of iron to 1 Gbar and 40, 000 K. Physical Review Letters, 2012, 108, 055505	7.4	70
91	First-principles calculation of the elastic moduli of sheet silicates and their application to shale anisotropy. <i>American Mineralogist</i> , <b>2011</b> , 96, 125-137	2.9	67
90	Calculated elastic constants and anisotropy of Mg2SiO4 spinel at high pressure. <i>Geophysical Research Letters</i> , <b>1997</b> , 24, 2841-2844	4.9	66
89	Atomic structure of SiO2 glass and its response to pressure. <i>Physical Review B</i> , <b>1991</b> , 44, 2523-2534	3.3	64
88	Phase stability and shear softening in CaSiO3 perovskite at high pressure. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	62
87	Constraints on the crystalline structure of the inner core: Mechanical instability of BCC iron at high pressure. <i>Geophysical Research Letters</i> , <b>1995</b> , 22, 125-128	4.9	59
86	First principles molecular dynamics simulations of diopside (CaMgSi2O6) liquid to high pressure. <i>Geochimica Et Cosmochimica Acta</i> , <b>2011</b> , 75, 3792-3802	5.5	56
85	First-principles calculations of the structural, dynamical, and electronic properties of liquid MgO. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	56
84	High-pressure proton disorder in brucite. <i>American Mineralogist</i> , <b>2006</b> , 91, 127-134	2.9	54
83	Bone chemical structure response to mechanical stress studied by high pressure Raman spectroscopy. <i>Calcified Tissue International</i> , <b>2005</b> , 76, 207-13	3.9	52
82	Elastic properties of MgSiO3-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
81	Absence of lattice strain anomalies at the electronic topological transition in zinc at high pressure. <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	49

## (2015-2014)

80	First-principles molecular dynamics simulations of MgSiO3 glass: Structure, density, and elasticity at high pressure. <i>American Mineralogist</i> , <b>2014</b> , 99, 1304-1314	2.9	46	
79	Magnetism in iron as a function of pressure. <i>Journal of Physics Condensed Matter</i> , <b>2004</b> , 16, S1109-S111	<b>9</b> 1.8	46	
78	Fluid helium at conditions of giant planetary interiors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2008</b> , 105, 11071-11075	11.5	42	
77	Inferring the thermochemical structure of the upper mantle from seismic data. <i>Geophysical Journal International</i> , <b>2009</b> , 179, 1169-1185	2.6	41	
76	Simple covalent potential models of tetrahedral SiO2: Applications to Equartz and coesite at pressure. <i>Physics and Chemistry of Minerals</i> , <b>1988</b> , 16, 199	1.6	41	
75	Spin crossover in ferropericlase from first-principles molecular dynamics. <i>Physical Review Letters</i> , <b>2015</b> , 114, 117202	7.4	40	
74	Melting in super-earths. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , <b>2014</b> , 372, 20130076	3	40	
73	Theoretical Methods for Calculating the Lattice Thermal Conductivity of Minerals. <i>Reviews in Mineralogy and Geochemistry</i> , <b>2010</b> , 71, 253-269	7.1	39	
72	First-principles study of diffusion and viscosity of anorthite (CaAl2Si2O8) liquid at high pressure. <i>American Mineralogist</i> , <b>2011</b> , 96, 744-751	2.9	39	
71	Visualization-based analysis of structural and dynamical properties of simulated hydrous silicate melt. <i>Physics and Chemistry of Minerals</i> , <b>2010</b> , 37, 103-117	1.6	39	
70	Structure and elasticity of wadsleyite at high pressures. <i>American Mineralogist</i> , <b>2001</b> , 86, 1387-1395	2.9	39	
69	Elastic constants and anisotropy of forsterite at high pressure. <i>Geophysical Research Letters</i> , <b>1997</b> , 24, 1963-1966	4.9	34	
68	Petrological interpretation of deep crustal intrusive bodies beneath oceanic hotspot provinces. <i>Geochemistry, Geophysics, Geosystems</i> , <b>2013</b> , 14, 604-619	3.6	33	
67	First-principles study of enhancement of transport properties of silica melt by water. <i>Physical Review Letters</i> , <b>2010</b> , 104, 215901	7.4	33	
66	A novel topological compression mechanism in a covalent liquid. <i>Science</i> , <b>1990</b> , 250, 541-3	33.3	33	
65	Al2O3 incorporation in MgSiO3 perovskite and ilmenite. <i>Earth and Planetary Science Letters</i> , <b>2006</b> , 252, 152-161	5.3	32	
64	Determination of the high-pressure properties of fayalite from first-principles calculations. <i>Earth and Planetary Science Letters</i> , <b>2010</b> , 289, 449-456	5.3	31	
63	First-principles calculations of the lattice thermal conductivity of the lower mantle. <i>Earth and Planetary Science Letters</i> , <b>2015</b> , 427, 11-17	5.3	30	

62	Estimates of the transition zone temperature in a mechanically mixed upper mantle. <i>Earth and Planetary Science Letters</i> , <b>2009</b> , 277, 244-252	5.3	30
61	Seismic velocities of major silicate and oxide phases of the lower mantle. <i>Journal of Geophysical Research</i> , <b>1999</b> , 104, 13025-13033		29
60	Primordial metallic melt in the deep mantle. <i>Geophysical Research Letters</i> , <b>2016</b> , 43, 3693-3699	4.9	29
59	Multidisciplinary Constraints on the Abundance of Diamond and Eclogite in the Cratonic Lithosphere. <i>Geochemistry, Geophysics, Geosystems</i> , <b>2018</b> , 19, 2062-2086	3.6	27
58	Akimotoite to perovskite phase transition in MgSiO3. <i>Geophysical Research Letters</i> , <b>2004</b> , 31, n/a-n/a	4.9	27
57	Elastic constants and anisotropy of MgSiO3 perovskite, periclase, and SiO2 at high pressure. <i>Geodynamic Series</i> , <b>1998</b> , 83-96		27
56	The EChO science case. Experimental Astronomy, 2015, 40, 329-391	1.3	26
55	Crystal chemistry of forsterite; a first-principles study. <i>American Mineralogist</i> , <b>1997</b> , 82, 663-671	2.9	26
54	The 10 mphase at high pressure by first principles calculations and implications for the petrology of subduction zones. <i>Earth and Planetary Science Letters</i> , <b>2007</b> , 260, 212-226	5.3	26
53	Electrical conductivity of SiO at extreme conditions and planetary dynamos. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2017</b> , 114, 9009-9013	11.5	25
52	Ab initio study of the elastic behavior of MgSiO3 ilmenite at high pressure. <i>Geophysical Research Letters</i> , <b>1999</b> , 26, 943-946	4.9	25
51	Spin crossover in Fe2SiO4 liquid at high pressure. <i>Geophysical Research Letters</i> , <b>2014</b> , 41, 4512-4518	4.9	24
50	Talc under tension and compression: Spinodal instability, elasticity, and structure. <i>Journal of Geophysical Research</i> , <b>2002</b> , 107, ECV 2-1-ECV 2-10		22
49	Extrinsic Elastic Anisotropy in a Compositionally Heterogeneous Earthß Mantle. <i>Journal of Geophysical Research: Solid Earth</i> , <b>2019</b> , 124, 1671-1687	3.6	20
48	A silicate dynamo in the early Earth. <i>Nature Communications</i> , <b>2020</b> , 11, 935	17.4	19
47	First principles viscosity and derived models for MgO-SiO2 melt system at high temperature. <i>Geophysical Research Letters</i> , <b>2013</b> , 40, 94-99	4.9	19
46	Normal and inverse ringwoodite at high pressures. American Mineralogist, 1999, 84, 288-293	2.9	18
45	Magnetic excitations and heat capacity of fayalite, Fe2SiO4. <i>American Mineralogist</i> , <b>2007</b> , 92, 481-490	2.9	17

44	Inner core anisotropy, anomalies in the time-averaged paleomagnetic field, and polarity transition paths. <i>Earth and Planetary Science Letters</i> , <b>1995</b> , 130, 75-85	5.3	17
43	Thermodynamics of the Earth® Mantle. Reviews in Mineralogy and Geochemistry, 2010, 71, 465-484	7.1	16
42	Energetics, equation of state, and elasticity of NAL phase: Potential host for alkali and aluminum in the lower mantle. <i>Geophysical Research Letters</i> , <b>2012</b> , 39, n/a-n/a	4.9	15
41	Joint mineral physics and seismic wave traveltime analysis of upper mantle temperature. <i>Geology</i> , <b>2009</b> , 37, 363-366	5	14
40	Chapter 19. THEORY OF MINERALS AT HIGH PRESSURE <b>1998</b> , 639-672		14
39	Stability of iron crystal structures at 0.3¶.5 TPa. Earth and Planetary Science Letters, 2015, 409, 299-306	5.3	13
38	Electronic conductivity of solid and liquid (Mg, Fe)O computed from first principles. <i>Earth and Planetary Science Letters</i> , <b>2018</b> , 490, 11-19	5.3	13
37	Spin crossover in liquid (Mg,Fe)O at extreme conditions. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	12
36	Theoretical Computation of Diffusion in Minerals and Melts. <i>Reviews in Mineralogy and Geochemistry</i> , <b>2010</b> , 72, 971-996	7.1	12
35	First-principles energetics and structural relaxation of antigorite. <i>American Mineralogist</i> , <b>2009</b> , 94, 1271	-1278	12
34	Stability of the hcp phase and temperature variation of the axial ratio of iron near Earth-core conditions. <i>Journal of Physics Condensed Matter</i> , <b>2007</b> , 19, 016208	1.8	12
33	Stability of (Mg,Fe)SiO3 perovskite and the structure of the lowermost mantle. <i>Geophysical Research Letters</i> , <b>1992</b> , 19, 1057-1060	4.9	12
32	Constraining the Volume of Earthß Early Oceans With a Temperature-Dependent Mantle Water Storage Capacity Model. <i>AGU Advances</i> , <b>2021</b> , 2, e2020AV000323	5.4	12
31	Critical vaporization of MgSiO. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2018</b> , 115, 5371-5376	11.5	11
30	Thermodynamic Analysis of the System MgO-FeO-SiO2 at High Pressure and the Structure of the Lowermost Mantle. <i>Geophysical Monograph Series</i> , <b>2013</b> , 131-141	1.1	11
29	A first-principle investigation of antigorite up to 30 GPa: Structural behavior under compression. <i>American Mineralogist</i> , <b>2012</b> , 97, 1177-1186	2.9	11
28	Measuring the melting curve of iron at super-Earth core conditions <i>Science</i> , <b>2022</b> , 375, 202-205	33.3	10
27	Density and Elasticity of Model Upper Mantle Compositions and their Implications for Whole Mantle Structure. <i>Geophysical Monograph Series</i> ,111-130	1.1	10

26	New high-pressure phases in MOOH (M = Al, Ga, In). <i>American Mineralogist</i> , <b>2018</b> , 103, 1906-1917	2.9	10
25	Compression of tetrahedrally bonded SIO2 liquid and silicate liquid-crystal density inversion. <i>Geophysical Research Letters</i> , <b>1989</b> , 16, 1403-1406	4.9	9
24	The top-down crystallisation of Mercury® core. Earth and Planetary Science Letters, 2019, 528, 115838	5.3	8
23	Heat and charge transport in HO at ice-giant conditions from ab initio molecular dynamics simulations. <i>Nature Communications</i> , <b>2020</b> , 11, 3605	17.4	8
22	Oceanic plateau of the Hawaiian mantle plume head subducted to the uppermost lower mantle. <i>Science</i> , <b>2020</b> , 370, 983-987	33.3	8
21	Physical properties of iron in the inner core. <i>Geodynamic Series</i> , <b>2003</b> , 137-161		7
20	Space <b>l</b> ime multiresolution atomistic visualization of MgO and MgSiO3 liquid data. <i>Visual Geosciences</i> , <b>2007</b> , 11, 1-11		6
19	Melting of CaSiO Perovskite at High Pressure. <i>Geophysical Research Letters</i> , <b>2019</b> , 46, 2037-2044	4.9	6
18	Elasticity of mantle phases at high pressure and temperature. <i>Geophysical Monograph Series</i> , <b>2000</b> , 201	-2₁1-3	5
17	First Principles Theory of Mantle and Core Phases. <i>Reviews in Mineralogy and Geochemistry</i> , <b>2001</b> , 42, 319-343	7.1	5
16	Thermal and Tidal Evolution of Uranus with a Growing Frozen Core. <i>Planetary Science Journal</i> , <b>2021</b> , 2, 222	2.9	5
15	Deep fractionation of Hf in a solidifying magma ocean and its implications for tungsten isotopic heterogeneities in the mantle. <i>Earth and Planetary Science Letters</i> , <b>2021</b> , 562, 116873	5.3	4
14	Thermal Conductivity of Silicate Liquid Determined by Machine Learning Potentials. <i>Geophysical Research Letters</i> , <b>2021</b> , 48, e2021GL093806	4.9	4
13	Advances in high-pressure mineral physics: From the deep mantle to the core. <i>Physics of the Earth and Planetary Interiors</i> , <b>2009</b> , 174, 1-2	2.3	3
12	The science of EChO. <i>Proceedings of the International Astronomical Union</i> , <b>2010</b> , 6, 359-370	0.1	3
11	First-Principles Investigations of Solid Iron at High Pressure and Implications for the Earth <b>ß</b> Inner Core. <i>Geophysical Monograph Series</i> , <b>1998</b> , 159-171	1.1	3
10	Mineral physics of the mantle. <i>Reviews of Geophysics</i> , <b>1995</b> , 33, 425	23.1	3
9	Thermal expansivity, heat capacity and bulk modulus of the mantle. <i>Geophysical Journal International</i> ,	2.6	3

8	9. First Principles Theory of Mantle and Core Phases <b>2001</b> , 319-344		2
7	Elasticity of Oxides and Ionics <b>2001</b> , 31-56		2
6	Entropy, dynamics, and freezing of CaSiO3 liquid. <i>Geochimica Et Cosmochimica Acta</i> , <b>2021</b> , 302, 1-17	5.5	2
5	22. Theoretical Computation of Diffusion in Minerals and Melts <b>2010</b> , 971-996		
4	Ab Initio Investigation of the High Pressure Elasticity of Mg2SiO4 Forsterite and Ringwoodite. <i>Materials Research Society Symposia Proceedings</i> , <b>1997</b> , 499, 15		
3	Elasticity, Thermal Properties, and Molecular Dynamics Using Non-Empirical Tight-Binding. <i>Materials Research Society Symposia Proceedings</i> , <b>1997</b> , 491, 501		
2	Thermoelastic Properties of (Mg,Fe)SiO3 Perovskite. <i>Materials Research Society Symposia Proceedings</i> , <b>2002</b> , 718, 1		
1	Water storage capacity of the Martian mantle through time. <i>Icarus</i> , <b>2022</b> , 115113	3.8	