Lindunka VoÄadlo

List of Publications by Year
in descending order

93	4,651	76326	98798
papers	citations	40 h-index	67 g-index

94	94	94	3116
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	ElasT: A toolkit for thermoelastic calculations. Computer Physics Communications, 2022, 273, 108280.	7.5	3
2	The effect of water on the outer core transport properties. Physics of the Earth and Planetary Interiors, 2022, 329-330, 106907.	1.9	3
3	Primitive noble gases sampled from ocean island basalts cannot be from the Earthâ€™s core. Nature Communications, 2022, 13, .	12.8	6
4	Equation of state for CO and CO2 fluids and their application on decarbonation reactions at high pressure and temperature. Chemical Geology, 2021, 559, 119918.	3.3	0
5	Strong shear softening induced by superionic hydrogen in Earth's inner core. Earth and Planetary Science Letters, 2021, 568, 117014.	4.4	29
6	Light elements in the Earthâ€™s core. Nature Reviews Earth & Environment, 2021, 2, 645-658.	29.7	69
7	Atomic transport properties of liquid iron at conditions of planetary cores. Journal of Chemical Physics, 2021, 155, 194505.	3.0	9
8	Equation of State of hcp Feâ€Câ€Si Alloys and the Effect of C Incorporation Mechanism on the Density of hcp Fe Alloys at 300ÂK. Journal of Geophysical Research: Solid Earth, 2020, 125, e2020JB020159.	3.4	10
9	The Earthâ€™s core as a reservoir of water. Nature Geoscience, 2020, 13, 453-458.	12.9	56
10	The top-down crystallisation of Mercury's core. Earth and Planetary Science Letters, 2019, 528, 115838.	4.4	11
11	Anisotropic diffusion creep in postperovskite provides a new model for deformation at the coreâ^'mantle boundary. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26389-26393.	7.1	7
12	Carbon Partitioning Between the Earth's Inner and Outer Core. Journal of Geophysical Research: Solid Earth, 2019, 124, 12812-12824.	3.4	23
13	Mg partitioning between solid and liquid iron under the Earthâ€™s core conditions. Physics of the Earth and Planetary Interiors, 2018, 274, 218-221.	1.9	8
14	The phase diagrams of KCaF3 and NaMgF3 by ab initio simulations. Physics and Chemistry of Minerals, 2018, 45, 311-322.	0.8	15
15	Melting properties from ab initio free energy calculations: Iron at the Earth's inner-core boundary. Physical Review B, 2018, 98, .	3.2	43
16	The thermal expansion of gold: point defect concentrations and pre-melting in a face-centred cubic metal. Journal of Applied Crystallography, 2018, 51, 470-480.	4.5	41
17	The elastic properties of hcp-Fe alloys under the conditions of the Earth's inner core. Earth and Planetary Science Letters, 2018, 493, 118-127.	4.4	59
18	High-temperature ab initio calculations on FeSi and NiSi at conditions relevant to small planetary cores. Physics and Chemistry of Minerals, 2017, 44, 477-484.	0.8	7

#	Article	IF	Citations
19	The thermal expansion of (Fe_{1â^'y}Ni_y)Si. Journal of Physics Condensed Matter, 2017, 29, 335701.	1.8	5
20	The phase diagram of NiSi under the conditions of small planetary interiors. Physics of the Earth and Planetary Interiors, 2016, 261, 196-206.	1.9	8
21	The elastic properties of hcp-Fe 1â^'x Si x at Earth's inner-core conditions. Earth and Planetary Science Letters, 2016, 451, 89-96.	4.4	25
22	Thermoelasticity of Fe₇C₃ under inner core conditions. Journal of Geophysical Research: Solid Earth, 2016, 121, 5828-5837.	3.4	28
23	High pressure stability of the monosilicides of cobalt and the platinum group elements. Journal of Alloys and Compounds, 2015, 626, 375-380.	5.5	16
24	The elastic properties and stability of fcc-Fe and fcc-FeNi alloys at inner-core conditions. Geophysical Journal International, 2015, 202, 94-101.	2.4	16
25	The equation of state of thePmmnphase of NiSi. Journal of Applied Crystallography, 2015, 48, 1914-1920.	4.5	2
26	The melting curve of Ni to 1 Mbar. Earth and Planetary Science Letters, 2014, 408, 226-236.	4.4	55
27	The NiSi melting curve to 70GPa. Physics of the Earth and Planetary Interiors, 2014, 233, 13-23.	1.9	36
28	Pâ€“Vâ€“Tequation of state of synthetic mirabilite (Na₂SO₄Â·10D₂O) determined by powder neutron diffraction. Journal of Applied Crystallography, 2013, 46, 448-460.	4.5	14
29	Strong Premelting Effect in the Elastic Properties of hcp-Fe Under Inner-Core Conditions. Science, 2013, 342, 466-468.	12.6	95
30	Core composition revealed. Nature, 2013, 495, 177-178.	27.8	1
31	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 Feâ€“Ni alloys. Earth and Planetary Science Letters, 2013, 365, 143-151.	4.4	62
32	High-pressure phase transitions and equations of state in NiSi. III. A new high-pressure phase of NiSi. Journal of Applied Crystallography, 2013, 46, 14-24.	4.5	12
33	High-pressure phase transitions and equations of state in NiSi. I.Ab initiosimulations. Journal of Applied Crystallography, 2012, 45, 186-196.	4.5	13
34	High-pressure phase transitions and equations of state in NiSi. II. Experimental results. Journal of Applied Crystallography, 2012, 45, 726-737.	4.5	10
35	Thermoelastic properties and crystal structure of CaPtO₃post-perovskite from 0 to 9â€…GPa and from 2Âto 973â€…K. Journal of Applied Crystallography, 2011, 44, 999-1016.	4.5	10
36	Equation of state and pressure-induced structural changes in mirabilite (Na2SO4Â·10H2O) determined from ab initio density functional theory calculations. Physics and Chemistry of Minerals, 2010, 37, 265-282.	0.8	17

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37	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. Physics of the Earth and Planetary Interiors, 2010, 178, 2-7.	1.9	20
38	The isothermal equation of state of CaPtO3 post-perovskite to 40GPa. Physics of the Earth and Planetary Interiors, 2010, 182, 113-118.	1.9	12
39	The thermal expansion and crystal structure of mirabilite (Na2SO4Â·10D2O) from 4.2 to 300ÂK, determined by time-of-flight neutron powder diffraction. Physics and Chemistry of Minerals, 2009, 36, 29-46.	0.8	42
40	Phase behaviour and thermoelastic properties of perdeuterated ammonia hydrate and ice polymorphs from 0 to 2â€...GPa. Journal of Applied Crystallography, 2009, 42, 846-866.	4.5	32
41	Ab initio calculations of the elasticity of hcp-Fe as a function of temperature at inner-core pressure. Earth and Planetary Science Letters, 2009, 288, 534-538.	4.4	97
42	New Views of the Earthâ€™s Inner Core from Computational Mineral Physics. , 2009, , 397-412.		1
43	The long-term stability of a possible aqueous ammonium sulfate ocean inside Titan. Icarus, 2008, 197, 137-151.	2.5	69
44	Thermoelastic properties of magnesiowÃ¼stite, (Mg_{1â^'x}Fe_x)O: determination of the Andersonâ€“GrÃ¼neisen parameter by time-of-flight neutron powder diffraction at simultaneous high pressures and temperatures. Journal of Applied Crystallography, 2008, 41, 886-896.	4.5	15
45	The effect of silicon impurities on the phase diagram of iron and possible implications for the Earth's core structure. Journal of Physics and Chemistry of Solids, 2008, 69, 2177-2181.	4.0	26
46	Light elements in the core: Effects of impurities on the phase diagram of iron. Geophysical Research Letters, 2008, 35, .	4.0	38
47	The stability of bcc-Fe at high pressures and temperatures with respect to tetragonal strain. Physics of the Earth and Planetary Interiors, 2008, 170, 52-59.	1.9	34
48	Ab initio calculations on the free energy and high Pâ€“T elasticity of face-centred-cubic iron. Earth and Planetary Science Letters, 2008, 268, 444-449.	4.4	31
49	High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores. Earth and Planetary Science Letters, 2008, 272, 481-487.	4.4	50
50	Ab initio calculations of the elasticity of iron and iron alloys at inner core conditions: Evidence for a partially molten inner core?. Earth and Planetary Science Letters, 2007, 254, 227-232.	4.4	119
51	The high-pressure phase diagram of ammonia dihydrate. High Pressure Research, 2007, 27, 201-212.	1.2	57
52	Crystal structures and thermal expansion of Î±-MgSO4and Î²-MgSO4from 4.2 to 300â€...K by neutron powder diffraction. Journal of Applied Crystallography, 2007, 40, 761-770.	4.5	35
53	Ammonium sulfate on Titan: Possible origin and role in cryovolcanism. Icarus, 2007, 188, 139-153.	2.5	157
54	Melting curve of copper measured to 16ÂGPa using a multi-anvil press. High Pressure Research, 2006, 26, 185-191.	1.2	39

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55	An ab initio study of nickel substitution into iron. Earth and Planetary Science Letters, 2006, 248, 147-152.	4.4	18
56	First-principles modelling of Earth and planetary materials at high pressures and temperatures. Reports on Progress in Physics, 2006, 69, 2365-2441.	20.1	152
57	The thermoelastic properties of MgSO47D2O (epsomite) from powder neutron diffraction and ab initio calculation. European Journal of Mineralogy, 2006, 18, 449-462.	1.3	50
58	The incompressibility and thermal expansivity of D2O ice II determined by powder neutron diffraction. Journal of Applied Crystallography, 2005, 38, 612-618.	4.5	47
59	Ab initiomelting curve of copper by the phase coexistence approach. Journal of Chemical Physics, 2004, 120, 2872-2878.	3.0	68
60	An ab initio study of the relative stabilities and equations of state of Fe3S polymorphs. Mineralogical Magazine, 2004, 68, 813-817.	1.4	6
61	Thermal expansion and crystal structure of cementite, Fe3C, between 4 and 600â€…K determined by time-of-flight neutron powder diffraction. Journal of Applied Crystallography, 2004, 37, 82-90.	4.5	186
62	Melting curve of materials: theory versus experiments. Journal of Physics Condensed Matter, 2004, 16, S973-S982.	1.8	59
63	The structure, ordering and equation of state of ammonia dihydrate (nh3 Â· 2h2o). Icarus, 2003, 162, 59-73.	2.5	30
64	Possible thermal and chemical stabilization of body-centred-cubic iron in the Earth's core. Nature, 2003, 424, 536-539.	27.8	249
65	Ab initio simulation of the ice II structure. Journal of Chemical Physics, 2003, 119, 4567-4572.	3.0	28
66	The equation of state of CsCl-structured FeSi to 40 GPa: Implications for silicon in the Earth's core. Geophysical Research Letters, 2003, 30, 14-1-14-4.	4.0	59
67	The properties of iron under core conditions from first principles calculations. Physics of the Earth and Planetary Interiors, 2003, 140, 101-125.	1.9	138
68	Hydrogen bonding in solid ammonia fromab initiocalculations. Journal of Chemical Physics, 2003, 118, 5987-5994.	3.0	47
69	A high-resolution neutron powder diffraction study of ammonia dihydrate (ND3â‹…2D2O) phase I. Journal of Chemical Physics, 2003, 119, 10806-10813.	3.0	37
70	A new high-pressure phase of FeSi. American Mineralogist, 2002, 87, 784-787.	1.9	72
71	The effect of ferromagnetism on the equation of state of Fe 3 C studied by first-principles calculations. Earth and Planetary Science Letters, 2002, 203, 567-575.	4.4	108
72	Thermal expansion and crystal structure of FeSi between 4 and 1173 K determined by time-of-flight neutron powder diffraction. Physics and Chemistry of Minerals, 2002, 29, 132-139.	0.8	113

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73	Ab initiomelting curve of the fcc phase of aluminum. Physical Review B, 2002, 65, .	3.2	124
74	Phonon Density of States of Iron up to 153 Gigapascals. Science, 2001, 292, 914-916.	12.6	284
75	Experimental verification of the Stokes-Einstein relation in liquid Feâ€”FeS at 5 GPa. Molecular Physics, 2001, 99, 773-777.	1.7	21
76	An ab initio study of the relative stabilities and equations of state of FeS polymorphs. Mineralogical Magazine, 2001, 65, 181-191.	1.4	21
77	Ab initio simulation of ammonia monohydrate (NH3â‹…H2O) and ammonium hydroxide (NH4OH). Journal of Chemical Physics, 2001, 115, 7006-7014.	3.0	44
78	In situ measurement of viscosity of liquids in the Fe-FeS system at high pressures and temperatures. American Mineralogist, 2000, 85, 1838-1842.	1.9	101
79	Structures and physical properties of â^Š-FeSi-type and CsCl-type RuSi studied by first-principles pseudopotential calculations. Acta Crystallographica Section B: Structural Science, 2000, 56, 369-376.	1.8	16
80	GrÃ¼neisen parameters and isothermal equations of state. American Mineralogist, 2000, 85, 390-395.	1.9	70
81	First principles calculations on the diffusivity and viscosity of liquid Feâ€“S at experimentally accessible conditions. Physics of the Earth and Planetary Interiors, 2000, 120, 145-152.	1.9	58
82	Ab initio free energy calculations on the polymorphs of iron at core conditions. Physics of the Earth and Planetary Interiors, 2000, 117, 123-137.	1.9	89
83	Crystal structure, compressibility and possible phase transitions in oldvarepsilon-FeSi studied by first-principles pseudopotential calculations. Acta Crystallographica Section B: Structural Science, 1999, 55, 484-493.	1.8	107
84	The Earth's deep interior: advances in theory and experiment. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 1999, 357, 3335-3357.	3.4	6
85	The structure of iron under the conditions of the Earth's inner core. Geophysical Research Letters, 1999, 26, 1231-1234.	4.0	47
86	First principles calculations on the high-pressure behavior of magnesite. American Mineralogist, 1999, 84, 1627-1631.	1.9	14
87	The Theory and Simulation of the Melting of Minerals. , 1999, , 561-575.		1
88	The viscosity of liquid iron at the physical conditions of the Earth's core. Nature, 1998, 392, 805-807.	27.8	259
89	First principles calculations on crystalline and liquid iron at Earth's core conditions. Faraday Discussions, 1997, 106, 205-218.	3.2	106
90	The melting of MgO â€” computer calculations via molecular dynamics. Physics and Chemistry of Minerals, 1996, 23, 42-49.	0.8	64

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91	Absolute ionic diffusion in MgOâ€"computer calculations via lattice dynamics. Physics of the Earth and Planetary Interiors, 1995, 88, 193-210.	1.9	44
92	Molecular dynamics: some recent developments in classical and quantum mechanical simulation of minerals. Mineralogical Magazine, 1995, 59, 597-605.	1.4	7
93	Thermal Properties of Liquid Iron at Conditions of Planetary Cores. Journal of Geophysical Research E: Planets, 0, , .	3.6	3