Gerd Steinle-Neumann

List of Publications by Year
in descending order

68 papers	2,963 citations	186209 28 h-index	168321 53 g-index
71 all docs	71 docs citations	71 times ranked	3584 citing authors

#	Article	IF	Citations
1	Possible Control of Earth's Boron Budget by Metallic Iron. Geophysical Research Letters, 2022, 49, .	1.5	3
2	Bulk modulus of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math> across the ice VIIâ€“ice X transition measured by time-resolved x-ray diffraction in dynamic diamond anvil cell experiments. Physical Review B, 2021, 103, .	1.1	24
3	Experimental determination of carbon diffusion in liquid iron at high pressure. American Mineralogist, 2021, , .	0.9	1
4	Anharmonic effects on the dynamics of solid aluminium from ab initio simulations. Journal of Physics Condensed Matter, 2021, 33, 175501.	0.7	3
5	Modeling the Viscosity of Anhydrous and Hydrous Volcanic Melts. Geochemistry, Geophysics, Geosystems, 2021, 22, e2021GC009918.	1.0	9
6	Synthesis of Ilmenite-type Îµ-Mn2O3 and Its Properties. Inorganic Chemistry, 2021, 60, 13348-13358.	1.9	4
7	Absence of proton tunneling during the hydrogen-bond symmetrization in Î´â^'AlOOH. Physical Review B, 2021, 104, .	1.1	7
8	The Helium Elemental and Isotopic Compositions of the Earth's Core Based on Ab Initio Simulations. Journal of Geophysical Research: Solid Earth, 2021, 126, e2021JB023106.	1.4	6
9	Lower Mantle Melting: Experiments and Thermodynamic Modeling in the System MgOâ€“SiO₂. Journal of Geophysical Research: Solid Earth, 2021, 126, e2021JB022568.	1.4	2
10	Structure and Density of H₂Oâ€Rich Mg₂SiO₄ Melts at High Pressure From Ab Initio Simulations. Journal of Geophysical Research: Solid Earth, 2020, 125, e2020JB020365.	1.4	10
11	Proton dynamics in high-pressure ice-VII from density functional theory. Physical Review B, 2020, 102, .	1.1	12
12	Proton mobility in metallic copper hydride from high-pressure nuclear magnetic resonance. Physical Review B, 2020, 102, .	1.1	14
13	Strong Sequestration of Hydrogen Into the Earth's Core During Planetary Differentiation. Geophysical Research Letters, 2020, 47, e2020GL088303.	1.5	31
14	Resistivity saturation in liquid ironâ€“light-element alloys at conditions of planetary cores from first principles computations. Comptes Rendus - Geoscience, 2019, 351, 154-162.	0.4	17
15	Pressure-Induced Hydrogen-Hydrogen Interaction in Metallic FeH Revealed by NMR. Physical Review X, 2019, 9, .	2.8	16
16	Mass Transport and Structural Properties of Binary Liquid Iron Alloys at High Pressure. Geochemistry, Geophysics, Geosystems, 2019, 20, 3556-3568.	1.0	12
17	Paramagnetic-to-Diamagnetic Transition in Dense Liquid Iron and Its Influence on Electronic Transport Properties. Physical Review Letters, 2019, 122, 086601.	2.9	17
18	Liquid Iron Equation of State to the Terapascal Regime From Ab Initio Simulations. Journal of Geophysical Research: Solid Earth, 2019, 124, 3350-3364.	1.4	23

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19	Electrical resistivity discontinuity of iron along the melting curve. Geophysical Journal International, 2018, 213, 237-243.	1.0	19
20	Saturation and negative temperature coefficient of electrical resistivity in liquid iron-sulfur alloys at high densities from first-principles calculations. Physical Review B, 2018, 97, .	1.1	18
21	A new ab initio equation of state of hcp-Fe and its implication on the interior structure and mass-radius relations of rocky super-Earths. Icarus, 2018, 313, 61-78.	1.1	66
22	Experimental determination of oxygen diffusion in liquid iron at high pressure. Earth and Planetary Science Letters, 2017, 464, 116-123.	1.8	20
23	Structural changes and anomalous selfâ€diffusion of oxygen in liquid iron at high pressure. Geophysical Research Letters, 2017, 44, 3526-3534.	1.5	15
24	High Pâ€“T experiments and first principles calculations of the diffusion of Si and Cr in liquid iron. Geochimica Et Cosmochimica Acta, 2017, 203, 323-342.	1.6	16
25	MMAâ€EoS: A Computational Framework for Mineralogical Thermodynamics. Journal of Geophysical Research: Solid Earth, 2017, 122, 9881-9920.	1.4	24
26	Spontaneous Charge Carrier Localization in Extended One-Dimensional Systems. Physical Review Letters, 2016, 116, 186401.	2.9	13
27	Thermal effects of variable material properties and metamorphic reactions in a threeâ€component subducting slab. Journal of Geophysical Research: Solid Earth, 2015, 120, 6823-6845.	1.4	10
28	Transport properties of silicate melts. Reviews of Geophysics, 2015, 53, 715-744.	9.0	66
29	Improved ground-state electronic structure and optical dielectric constants with a semilocal exchange functional. Physical Review B, 2015, 91, .	1.1	19
30	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. Journal of Chemical Physics, 2015, 142, 034107.	1.2	42
31	Stability of MnB2 with AlB2-type structure revealed by first-principles calculations and experiments. Applied Physics Letters, 2013, 102, .	1.5	14
32	Electrical resistivity and thermal conductivity of liquid Fe alloys at high P and T , and heat flux in Earthâ€™s core. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 4070-4073.	3.3	268
33	The effect of variable thermal diffusivity on kinematic models of subduction. Journal of Geophysical Research, 2012, 117, .	3.3	16
34	Electrical and thermal conductivity of Al liquid at high pressures and temperatures fromab initiocomputations. Physical Review B, 2012, 85, .	1.1	37
35	High-pressure behavior of iron carbide (Fe₇C₃) at inner core conditions. Journal of Geophysical Research, 2011, 116, .	3.3	75
36	Transport properties of Mg2SiO4 liquid at high pressure: Physical state of a magma ocean. Earth and Planetary Science Letters, 2011, 312, 463-470.	1.8	39

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37	In situhigh-pressure study of LiNbO₃-type FeTiO₃: X-ray diffraction and MÃ¶ssbauer spectroscopy. High Pressure Research, 2010, 30, 395-405.	0.4	20
38	Structural stability of TiO2at high pressure in density-functional theory based calculations. Journal of Physics Condensed Matter, 2010, 22, 295501.	0.7	30
39	First-principles phase diagram calculations for the HfCâ€“TiC, ZrCâ€“TiC, and HfCâ€“ZrC solid solutions. Physical Review B, 2009, 80, .	1.1	65
40	Iron oxidation state of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>FeTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:m high pressure. Physical Review B, 2009, 79, .	3.1	29
41	Detecting deeply subducted crust from the elasticity of hollandite. Earth and Planetary Science Letters, 2009, 288, 349-358.	1.8	41
42	Ab initio predictions of potassium partitioning between Fe and Al-bearing MgSiO3 perovskite and post-perovskite. Physics of the Earth and Planetary Interiors, 2009, 174, 247-253.	0.7	7
43	Thermal versus elastic heterogeneity in highâ€resolution mantle circulation models with pyrolite composition: High plume excess temperatures in the lowermost mantle. Geochemistry, Geophysics, Geosystems, 2009, 10, .	1.0	111
44	Elasticity of phaseâ€X at high pressure. Geophysical Research Letters, 2009, 36, .	1.5	20
45	Pressure-induced phase transitions of AX₂-type iron pnictides: anab initiostudy. Journal of Physics Condensed Matter, 2009, 21, 185403.	0.7	17
46	Short-range order and Fe clustering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mg</mml:mtext></mml:mrow><mml:mrow><mml:mn> high pressure. Physical Review B, 2009, 80, .	1.1	44
47	Structural study of FeP2 at high pressure. High Pressure Research, 2009, 29, 235-244.	0.4	15
48	High-Pressure Behavior of Perovskite:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>FeTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Dissociation into<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo		

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55	Nonequivalence of the octahedral sites of cubicFe3O4magnetite. Physical Review B, 2007, 75, .	1.1	25
56	A mineralogical model for density and elasticity of the Earth's mantle. Geochemistry, Geophysics, Geosystems, 2007, 8, .	1.0	43
57	Ab-initio simulation of elastic constants for some ceramic materials. European Physical Journal B, 2007, 58, 127-133.	0.6	91
58	High-pressure alloying of iron and xenon: â€œMissingâ€•Xe in the Earth's core?. Journal of Geophysical Research, 2006, 111, n/a-n/a.	3.3	25
59	Compression Behavior of Zr-doped Nanoanatase. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2006, 61, 1577-1585.	0.3	7
60	Effect of Al on the sharpness of the MgSiO3perovskite to post-perovskite phase transition. Geophysical Research Letters, 2005, 32, n/a-n/a.	1.5	71
61	Magnetism in dense hexagonal iron. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 33-36.	3.3	87
62	Ab-initiohigh-pressure alloying of iron and potassium: Implications for the Earth's core. Geophysical Research Letters, 2004, 31, n/a-n/a.	1.5	33
63	Magnetism in iron as a function of pressure. Journal of Physics Condensed Matter, 2004, 16, S1109-S1119.	0.7	53
64	Comment on ÂOn the importance of the free energy for elasticity under pressureÂ. Journal of Physics Condensed Matter, 2004, 16, 8783-8786.	0.7	33
65	Physical properties of iron in the inner core. Geodynamic Series, 2003, , 137-161.	0.1	7
66	Elasticity of iron at the temperature of the Earth's inner core. Nature, 2001, 413, 57-60.	13.7	240
67	Absence of lattice strain anomalies at the electronic topological transition in zinc at high pressure. Physical Review B, 2001, 63, .	1.1	52
68	First-principles elastic constants for the hcp transition metals Fe, Co, and Re at high pressure. Physical Review B, 1999, 60, 791-799.	1.1	355