

# Gerd Steinle-Neumann

## List of Publications by Year in descending order

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Version: 2024-02-01

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	First-principles elastic constants for the hcp transition metals Fe, Co, and Re at high pressure. <i>Physical Review B</i> , 1999, 60, 791-799.	1.1	355
2	Electrical resistivity and thermal conductivity of liquid Fe alloys at high $P$ and $T$ , and heat flux in Earth's core. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 4070-4073.	3.3	268
3	The effect of valence state and site geometry on Ti L <sub>2,3</sub> and O K electron energy-loss spectra of Ti <sub>x</sub> O <sub>y</sub> phases. <i>American Mineralogist</i> , 2007, 92, 577-586.	0.9	265
4	Elasticity of iron at the temperature of the Earth's inner core. <i>Nature</i> , 2001, 413, 57-60.	13.7	240
5	Thermal versus elastic heterogeneity in high-resolution mantle circulation models with pyrolite composition: High plume excess temperatures in the lowermost mantle. <i>Geochemistry, Geophysics, Geosystems</i> , 2009, 10, .	1.0	111
6	Ab-initio simulation of elastic constants for some ceramic materials. <i>European Physical Journal B</i> , 2007, 58, 127-133.	0.6	91
7	Magnetism in dense hexagonal iron. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 33-36.	3.3	87
8	High-pressure behavior of iron carbide (Fe <sub>7</sub> C <sub>3</sub> ) at inner core conditions. <i>Journal of Geophysical Research</i> , 2011, 116, .	3.3	75
9	Effect of Al on the sharpness of the MgSiO <sub>3</sub> perovskite to post-perovskite phase transition. <i>Geophysical Research Letters</i> , 2005, 32, n/a-n/a.	1.5	71
10	Transport properties of silicate melts. <i>Reviews of Geophysics</i> , 2015, 53, 715-744.	9.0	66
11	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. <i>Icarus</i> , 2018, 313, 61-78.	1.1	66
12	First-principles phase diagram calculations for the HfC-TiC, ZrC-TiC, and HfC-ZrC solid solutions. <i>Physical Review B</i> , 2009, 80, .	1.1	65
13	Magnetism in iron as a function of pressure. <i>Journal of Physics Condensed Matter</i> , 2004, 16, S1109-S1119.	0.7	53
14	Absence of lattice strain anomalies at the electronic topological transition in zinc at high pressure. <i>Physical Review B</i> , 2001, 63, .	1.1	52
15	Mg <sub>2</sub> SiO <sub>4</sub> liquid under high pressure from molecular dynamics. <i>Chemical Geology</i> , 2008, 256, 185-192.	1.4	51
16	Short-range order and Fe clustering in $\text{Mg}_{1-x}\text{Fe}_x\text{O}$ under high pressure. <i>Physical Review B</i> , 2009, 80, .	1.1	44
17	A mineralogical model for density and elasticity of the Earth's mantle. <i>Geochemistry, Geophysics, Geosystems</i> , 2007, 8, .	1.0	43
18	Magnetism and the Verwey transition in $\text{Fe}_3\text{O}_4$ under pressure. <i>Physical Review B</i> , 2008, 77, .	1.1	42

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19	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. Journal of Chemical Physics, 2015, 142, 034107.	1.2	42
20	Detecting deeply subducted crust from the elasticity of hollandite. Earth and Planetary Science Letters, 2009, 288, 349-358.	1.8	41
21	Transport properties of Mg <sub>2</sub> SiO <sub>4</sub> liquid at high pressure: Physical state of a magma ocean. Earth and Planetary Science Letters, 2011, 312, 463-470.	1.8	39
22	Electrical and thermal conductivity of Al liquid at high pressures and temperatures from <i>ab initio</i> computations. Physical Review B, 2012, 85, .	1.1	37
23	<i>Ab-initio</i> high-pressure alloying of iron and potassium: Implications for the Earth's core. Geophysical Research Letters, 2004, 31, n/a-n/a.	1.5	33
24	Comment on "On the importance of the free energy for elasticity under pressure". Journal of Physics Condensed Matter, 2004, 16, 8783-8786.	0.7	33
25	Anomalous pressure evolution of the axial ratio $c/a$ in hcp cobalt: Interplay between structure, magnetism, and lattice dynamics. Applied Physics Letters, 2008, 92, .	1.5	31
26	Strong Sequestration of Hydrogen Into the Earth's Core During Planetary Differentiation. Geophysical Research Letters, 2020, 47, e2020GL088303.	1.5	31
27	Structural stability of TiO <sub>2</sub> at high pressure in density-functional theory based calculations. Journal of Physics Condensed Matter, 2010, 22, 295501.	0.7	30
28	Iron oxidation state of $\text{FeTiO}_3$ at high pressure. Physical Review B, 2009, 79, .	1.1	29
29	High-pressure alloying of iron and xenon: "Missing" Xe in the Earth's core?. Journal of Geophysical Research, 2006, 111, n/a-n/a.	3.3	25
30	Nonequivalence of the octahedral sites of cubic Fe <sub>3</sub> O <sub>4</sub> magnetite. Physical Review B, 2007, 75, .	1.1	25
31	MMA-EoS: A Computational Framework for Mineralogical Thermodynamics. Journal of Geophysical Research: Solid Earth, 2017, 122, 9881-9920.	1.4	24
32	Bulk modulus of $\text{H}_2\text{O}$ across the ice VII "ice X" transition measured by time-resolved x-ray diffraction in dynamic diamond anvil cell experiments. Physical Review B, 2021, 103, .	1.1	24
33	High-Pressure Behavior of Perovskite: $\text{FeTiO}_3$ Dissociation into $\text{FeTiO}_3$		

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37	Elasticity of phase $\epsilon$ at high pressure. <i>Geophysical Research Letters</i> , 2009, 36, .	1.5	20
38	<i>In situ</i> high-pressure study of $\text{LiNbO}_3$ -type $\text{FeTiO}_3$ : X-ray diffraction and Mössbauer spectroscopy. <i>High Pressure Research</i> , 2010, 30, 395-405.	0.4	20
39	Experimental determination of oxygen diffusion in liquid iron at high pressure. <i>Earth and Planetary Science Letters</i> , 2017, 464, 116-123.	1.8	20
40	Improved ground-state electronic structure and optical dielectric constants with a semilocal exchange functional. <i>Physical Review B</i> , 2015, 91, .	1.1	19
41	Electrical resistivity discontinuity of iron along the melting curve. <i>Geophysical Journal International</i> , 2018, 213, 237-243.	1.0	19
42	Saturation and negative temperature coefficient of electrical resistivity in liquid iron-sulfur alloys at high densities from first-principles calculations. <i>Physical Review B</i> , 2018, 97, .	1.1	18
43	Pressure-induced phase transitions of $\text{AX}_2$ -type iron pnictides: an <i>ab initio</i> study. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 185403.	0.7	17
44	Resistivity saturation in liquid iron–light-element alloys at conditions of planetary cores from first principles computations. <i>Comptes Rendus - Geoscience</i> , 2019, 351, 154-162.	0.4	17
45	Paramagnetic-to-Diamagnetic Transition in Dense Liquid Iron and Its Influence on Electronic Transport Properties. <i>Physical Review Letters</i> , 2019, 122, 086601.	2.9	17
46	The effect of variable thermal diffusivity on kinematic models of subduction. <i>Journal of Geophysical Research</i> , 2012, 117, .	3.3	16
47	High $P$ – $T$ experiments and first principles calculations of the diffusion of Si and Cr in liquid iron. <i>Geochimica Et Cosmochimica Acta</i> , 2017, 203, 323-342.	1.6	16
48	Pressure-Induced Hydrogen-Hydrogen Interaction in Metallic FeH Revealed by NMR. <i>Physical Review X</i> , 2019, 9, .	2.8	16
49	Structural study of $\text{FeP}_2$ at high pressure. <i>High Pressure Research</i> , 2009, 29, 235-244.	0.4	15
50	Structural changes and anomalous self-diffusion of oxygen in liquid iron at high pressure. <i>Geophysical Research Letters</i> , 2017, 44, 3526-3534.	1.5	15
51	Stability of $\text{MnB}_2$ with $\text{AlB}_2$ -type structure revealed by first-principles calculations and experiments. <i>Applied Physics Letters</i> , 2013, 102, .	1.5	14
52	Proton mobility in metallic copper hydride from high-pressure nuclear magnetic resonance. <i>Physical Review B</i> , 2020, 102, .	1.1	14
53	Spontaneous Charge Carrier Localization in Extended One-Dimensional Systems. <i>Physical Review Letters</i> , 2016, 116, 186401.	2.9	13
54	Mass Transport and Structural Properties of Binary Liquid Iron Alloys at High Pressure. <i>Geochemistry, Geophysics, Geosystems</i> , 2019, 20, 3556-3568.	1.0	12

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55	Proton dynamics in high-pressure ice-VII from density functional theory. <i>Physical Review B</i> , 2020, 102, .	1.1	12
56	Thermal effects of variable material properties and metamorphic reactions in a three-component subducting slab. <i>Journal of Geophysical Research: Solid Earth</i> , 2015, 120, 6823-6845.	1.4	10
57	Structure and Density of H <sub>2</sub> -Rich Mg <sub>2</sub> SiO <sub>4</sub> Melts at High Pressure From Ab Initio Simulations. <i>Journal of Geophysical Research: Solid Earth</i> , 2020, 125, e2020JB020365.	1.4	10
58	Modeling the Viscosity of Anhydrous and Hydrous Volcanic Melts. <i>Geochemistry, Geophysics, Geosystems</i> , 2021, 22, e2021GC009918.	1.0	9
59	Physical properties of iron in the inner core. <i>Geodynamic Series</i> , 2003, , 137-161.	0.1	7
60	Compression Behavior of Zr-doped Nanoanatase. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2006, 61, 1577-1585.	0.3	7
61	Ab initio predictions of potassium partitioning between Fe and Al-bearing MgSiO <sub>3</sub> perovskite and post-perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 2009, 174, 247-253.	0.7	7
62	Absence of proton tunneling during the hydrogen-bond symmetrization in $\gamma$ -AlOOH. <i>Physical Review B</i> , 2021, 104, .	1.1	7
63	The Helium Elemental and Isotopic Compositions of the Earth's Core Based on Ab Initio Simulations. <i>Journal of Geophysical Research: Solid Earth</i> , 2021, 126, e2021JB023106.	1.4	6
64	Synthesis of Ilmenite-type $\mu$ -Mn <sub>2</sub> O <sub>3</sub> and Its Properties. <i>Inorganic Chemistry</i> , 2021, 60, 13348-13358.	1.9	4
65	Anharmonic effects on the dynamics of solid aluminium from ab initio simulations. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 175501.	0.7	3
66	Possible Control of Earth's Boron Budget by Metallic Iron. <i>Geophysical Research Letters</i> , 2022, 49, .	1.5	3
67	Lower Mantle Melting: Experiments and Thermodynamic Modeling in the System MgO-SiO <sub>2</sub> . <i>Journal of Geophysical Research: Solid Earth</i> , 2021, 126, e2021JB022568.	1.4	2
68	Experimental determination of carbon diffusion in liquid iron at high pressure. <i>American Mineralogist</i> , 2021, , .	0.9	1