

Koichiro Umemoto

List of Publications by Year in descending order

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73
papers

3,315
citations

159358

30
h-index

143772

57
g-index

73
all docs

73
docs citations

73
times ranked

2728
citing authors

#	ARTICLE	IF	CITATIONS
1	Phase transition in MgSiO ₃ perovskite in the earth's lower mantle. Earth and Planetary Science Letters, 2004, 224, 241-248.	1.8	571
2	Body-Centered Tetragonal C_4 : A Viable Carbon Allotrope. Physical Review Letters, 2010, 104, 125504.	2.9	363
3	Dissociation of MgSiO ₃ in the Cores of Gas Giants and Terrestrial Exoplanets. Science, 2006, 311, 983-986.	6.0	166
4	Crystallization of silicon dioxide and compositional evolution of the Earth's core. Nature, 2017, 543, 99-102.	13.7	161
5	Elasticity of post-perovskite MgSiO ₃ . Geophysical Research Letters, 2004, 31, .	1.5	147
6	Spin states and hyperfine interactions of iron in (Mg,Fe)SiO ₃ perovskite under pressure. Earth and Planetary Science Letters, 2010, 294, 19-26.	1.8	102
7	First-principles study for low-spin $LaCoO_3$ a structurally consistent Hubbard U . Physical Review B, 2009, 79, .	1.1	100
8	Pressure-volume-temperature relations in MgO: An ultrahigh pressure-temperature scale for planetary sciences applications. Journal of Geophysical Research, 2008, 113, .	3.3	84
9	Co _{1-x} FexS ₂ : A Tunable Source of Highly Spin-Polarized Electrons. Physical Review Letters, 2005, 94, 056602.	2.9	77
10	Carbon foam: Spanning the phase space between graphite and diamond. Physical Review B, 2001, 64, .	1.1	74
11	Ultrahigh-pressure phases of H_2O ice predicted using an adaptive genetic algorithm. Physical Review B, 2011, 84, .	1.1	72
12	Spin transition in (Mg,Fe)SiO ₃ perovskite under pressure. Earth and Planetary Science Letters, 2008, 276, 198-206.	1.8	65
13	Liquid iron-hydrogen alloys at outer core conditions by first-principles calculations. Geophysical Research Letters, 2015, 42, 7513-7520.	1.5	64
14	Two-stage dissociation in MgSiO ₃ post-perovskite. Earth and Planetary Science Letters, 2011, 311, 225-229.	1.8	58
15	First principles investigation of the postspinel transition in Mg ₂ SiO ₄ . Geophysical Research Letters, 2007, 34, .	1.5	55
16	Prediction of an U_2S_3 -type polymorph of Al_2O_3 at 3.7 Mbar. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6526-6530.	3.3	55
17	A first-principles investigation of hydrous defects and IR frequencies in forsterite: The case for Si vacancies. American Mineralogist, 2011, 96, 1475-1479.	0.9	53
18	Lattice dynamics and thermal equation of state of platinum. Physical Review B, 2008, 78, .	1.1	47

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19	Identification of post-pyrite phase transitions in SiO ₂ by a genetic algorithm. <i>Physical Review B</i> , 2011, 83, .	1.1	46
20	Phase transitions in MgSiO ₃ post-perovskite in super-Earth mantles. <i>Earth and Planetary Science Letters</i> , 2017, 478, 40-45.	1.8	45
21	NaMgF ₃ : A low-pressure analog of MgSiO ₃ . <i>Geophysical Research Letters</i> , 2006, 33, .	1.5	43
22	Composition controlled spin polarization in Co _{1-x} Fe _x S ₂ : Electronic, magnetic, and thermodynamic properties. <i>Physical Review B</i> , 2006, 73, .	1.1	43
23	Order-disorder phase boundary between ice VII and VIII obtained by first principles. <i>Chemical Physics Letters</i> , 2010, 499, 236-240.	1.2	40
24	Composition controlled spin polarization in Co _{1-x} Fe _x S ₂ alloys. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 315219.	0.7	39
25	Spin-State Crossover of Iron in Lower-Mantle Minerals: Results of DFT+U Investigations. <i>Reviews in Mineralogy and Geochemistry</i> , 2010, 71, 169-199.	2.2	38
26	Liquid iron-sulfur alloys at outer core conditions by first-principles calculations. <i>Geophysical Research Letters</i> , 2014, 41, 6712-6717.	1.5	38
27	Anomalous Pressure-Induced Transition(s) in Ice XI. <i>Physical Review Letters</i> , 2004, 92, 105502.	2.9	37
28	Elasticity of diamond at high pressures and temperatures. <i>Applied Physics Letters</i> , 2012, 101, .	1.5	37
29	Chemical compositions of the outer core examined by first principles calculations. <i>Earth and Planetary Science Letters</i> , 2020, 531, 116009.	1.8	37
30	Glycine Polymerization on Oxide Minerals. <i>Origins of Life and Evolution of Biospheres</i> , 2017, 47, 123-143.	0.8	36
31	Effect of the d electrons on phase transitions in transition-metal sesquioxides. <i>Physics and Chemistry of Minerals</i> , 2011, 38, 387-395.	0.3	31
32	Effect of site degeneracies on the spin crossovers in (Mg, Fe)SiO ₃ perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 2010, 180, 209-214.	0.7	27
33	The Hubbard U correction for iron-bearing minerals: A discussion based on (Mg,Fe)SiO ₃ perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 2011, 185, 13-19.	0.7	27
34	Mass-dependent dynamics of terrestrial exoplanets using ab initio mineral properties. <i>Icarus</i> , 2019, 317, 412-426.	1.1	27
35	Potential ultrahigh pressure polymorphs of ABX ₃ -type compounds. <i>Physical Review B</i> , 2006, 74, .	1.1	26
36	Electronic Configurations of Superheavy Elements. <i>Journal of the Physical Society of Japan</i> , 1996, 65, 3175-3179.	0.7	25

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37	Electronic structure of Co _{1-x} Fe _x S ₂ . <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 2117-2121.	0.7	25
38	Stability of fcc phase FeH to 137 GPa. <i>American Mineralogist</i> , 2020, 105, 917-921.	0.9	25
39	Theoretical study of the isostructural transformation in ice VIII. <i>Physical Review B</i> , 2005, 71, .	1.1	24
40	Nature of the Volume Isotope Effect in Ice. <i>Physical Review Letters</i> , 2015, 115, 173005.	2.9	22
41	Post-stishovite transition in hydrous aluminous SiO ₂ . <i>Physics of the Earth and Planetary Interiors</i> , 2016, 255, 18-26.	0.7	21
42	Phase transition in SiC from zinc-blende to rock-salt structure and implications for carbon-rich extrasolar planets. <i>American Mineralogist</i> , 2017, 102, 2230-2234.	0.9	21
43	qha: A Python package for quasiharmonic free energy calculation for multi-configuration systems. <i>Computer Physics Communications</i> , 2019, 237, 199-207.	3.0	21
44	Amorphization in quenched ice VIII: A first-principles study. <i>Physical Review B</i> , 2004, 69, .	1.1	20
45	Fundamentals of elasticity of (Mg _{1-x} Fe _x) ₂ TiO ₄ . <i>Journal of Applied Physics</i> , 2015, 118, 045101.	1.5	19
46	Ab initio study of water speciation in forsterite: Importance of the entropic effect. <i>American Mineralogist</i> , 2018, 103, 692-699.	0.9	18
47	Electronic structure of the Ba ₄ C ₆ O superconductor. <i>Physical Review B</i> , 2000, 61, 14204-14208.	1.1	15
48	First-principles studies of spin-state crossovers of iron in perovskite. <i>European Journal of Mineralogy</i> , 2012, 24, 851-862.	0.4	14
49	Electronic structure of K ₃ Ba ₃ C ₆ O and Rb ₃ Ba ₃ C ₆ O superconductors. <i>Physical Review B</i> , 1999, 60, 16186-16191.	1.1	13
50	Energetics and structural stability of Cs ₃ C ₆ O. <i>Solid State Communications</i> , 2004, 130, 335-339.	0.9	12
51	Multi-Mbar Phase Transitions in Minerals. <i>Reviews in Mineralogy and Geochemistry</i> , 2010, 71, 299-314.	2.2	10
52	Ab initio exploration of post-PPV transitions in low-pressure analogs of MgSiO ₃ . <i>Physical Review Materials</i> , 2019, 3, .	0.9	10
53	Hierarchical assembly of nanostructured carbon foam. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 386, 189-195.	0.4	9
54	Low-temperature high density transformations in ice. <i>Chemical Physics Letters</i> , 2005, 405, 53-57.	1.2	9

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55	Computer Simulations on Phase Transitions in Ice. <i>Reviews in Mineralogy and Geochemistry</i> , 2010, 71, 315-335.	2.2	9
56	First-Principles Determination of the Dissociation Phase Boundary of Phase H MgSiO ₄ . <i>Geophysical Research Letters</i> , 2019, 46, 7333-7336.	1.5	9
57	Melting phase relations in Fe-Si-H at high pressure and implications for Earth's inner core crystallization. <i>Scientific Reports</i> , 2022, 12, .	1.6	8
58	First principles study of volume isotope effects in ices VIII and X. <i>Japanese Journal of Applied Physics</i> , 2017, 56, 05FA03.	0.8	6
59	<i>Ab initio</i> prediction of an order-disorder transition in Mg ₂ O ₄ : Implication for the nature of super-Earth's mantles. <i>Physical Review Materials</i> , 2021, 5, .	0.9	5
60	<i>Ab initio</i> investigation of H-bond disordering in γ -AlOOH. <i>Physical Review Research</i> , 2022, 4, .	1.3	4
61	9. Spin-State Crossover of Iron in Lower-Mantle Minerals: Results of DFT+U Investigations. , 2010, , 169-200.		2
62	Correction to "Pressure-volume-temperature relations in MgO: An ultrahigh pressure-temperature scale for planetary sciences applications". <i>Journal of Geophysical Research</i> , 2010, 115, .	3.3	2
63	Structural transition and re-emergence of iron's total electron spin in (Mg,Fe)O at ultrahigh pressure. <i>Nature Communications</i> , 2022, 13, 2780.	5.8	2
64	Electronic Structure and Energetics of Fullerites, Fullerides, and Fullerene Polymers. <i>Structure and Bonding</i> , 0, , 41-57.	1.0	1
65	Thermodynamic Properties and Stability Field of MgSiO ₃ Post-Perovskite. <i>Geophysical Monograph Series</i> , 2007, , 79-97.	0.1	1
66	Searching for high magnetization density in bulk Fe: the new metastable Fe ₆ phase. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 016001.	0.7	1
67	Two-stages Dissociation of NaMgF ₃ Post-Perovskite: A Potential Low-Pressure Analog of MgSiO ₃ at Multi-Mbar Pressures. , 2015, , .		1
68	Electronic structure of body-centered lattice fullerides. <i>AIP Conference Proceedings</i> , 2000, , .	0.3	0
69	Hybridization between K and C ₆₀ Electronic States in Superconducting K ₃ Ba ₃ C ₆₀ . <i>Molecular Crystals and Liquid Crystals</i> , 2000, 340, 605-610.	0.3	0
70	Electronic structure of Ba ₄ C ₆₀ and Cs ₄ C ₆₀ . <i>AIP Conference Proceedings</i> , 2001, , .	0.3	0
71	15. Computer Simulations on Phase Transitions in Ice. , 2010, , 315-336.		0
72	14. Multi-Mbar Phase Transitions in Minerals. , 2010, , 299-314.		0

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73	First-Principles Study of Phase Transitions of Minerals in Super-Earths. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2017, 27, 205-212.	0.1	0