

Koichiro Umemoto

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

67
papers

2,735
citations

27
h-index

52
g-index

73
ext. papers

3,002
ext. citations

5.1
avg, IF

5.13
L-index

#	Paper	IF	Citations
67	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	17.4	
66	Stability of fcc phase FeH to 137 GPa. <i>American Mineralogist</i> , 2020 , 105, 917-921	2.9	8
65	Chemical compositions of the outer core examined by first principles calculations. <i>Earth and Planetary Science Letters</i> , 2020 , 531, 116009	5.3	18
64	First-Principles Determination of the Dissociation Phase Boundary of Phase H MgSiO ₄ H ₂ . <i>Geophysical Research Letters</i> , 2019 , 46, 7333-7336	4.9	5
63	Ab initio exploration of post-PPV transitions in low-pressure analogs of MgSiO ₃ . <i>Physical Review Materials</i> , 2019 , 3,	3.2	3
62	Mass-dependent dynamics of terrestrial exoplanets using ab initio mineral properties. <i>Icarus</i> , 2019 , 317, 412-426	3.8	11
61	qha: A Python package for quasiharmonic free energy calculation for multi-configuration systems. <i>Computer Physics Communications</i> , 2019 , 237, 199-207	4.2	6
60	Ab initio study of water speciation in forsterite: Importance of the entropic effect. <i>American Mineralogist</i> , 2018 , 103, 692-699	2.9	13
59	Crystallization of silicon dioxide and compositional evolution of the Earth's core. <i>Nature</i> , 2017 , 543, 99-102	32.4	120
58	First principles study of volume isotope effects in ices VIII and X. <i>Japanese Journal of Applied Physics</i> , 2017 , 56, 05FA03	1.4	6
57	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	2.9	15
56	Phase transitions in MgSiO ₃ post-perovskite in super-Earth mantles. <i>Earth and Planetary Science Letters</i> , 2017 , 478, 40-45	5.3	24
55	Glycine Polymerization on Oxide Minerals. <i>Origins of Life and Evolution of Biospheres</i> , 2017 , 47, 123-143	1.5	29
54	First-Principles Study of Phase Transitions of Minerals in Super-Earths. <i>Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu</i> , 2017 , 27, 205-212	0	
53	Post-stishovite transition in hydrous aluminous SiO ₂ . <i>Physics of the Earth and Planetary Interiors</i> , 2016 , 255, 18-26	2.3	14
52	Two-stages Dissociation of NaMgF ₃ Post-Perovskite: A Potential Low-Pressure Analog of MgSiO ₃ at Multi-Mbar Pressures 2015 ,		1
51	Nature of the Volume Isotope Effect in Ice. <i>Physical Review Letters</i> , 2015 , 115, 173005	7.4	17

50	Liquid iron-hydrogen alloys at outer core conditions by first-principles calculations. <i>Geophysical Research Letters</i> , 2015 , 42, 7513-7520	4.9	46
49	Searching for high magnetization density in bulk Fe: the new metastable Fe β phase. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 016001	1.8	1
48	Liquid iron-sulfur alloys at outer core conditions by first-principles calculations. <i>Geophysical Research Letters</i> , 2014 , 41, 6712-6717	4.9	34
47	Elasticity of diamond at high pressures and temperatures. <i>Applied Physics Letters</i> , 2012 , 101, 171902	3.4	27
46	First-principles studies of spin-state crossovers of iron in perovskite. <i>European Journal of Mineralogy</i> , 2012 , 24, 851-862	2.2	14
45	Two-stage dissociation in MgSiO ₃ post-perovskite. <i>Earth and Planetary Science Letters</i> , 2011 , 311, 225-229	3.3	49
44	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	2.3	21
43	Effect of the d electrons on phase transitions in transition-metal sesquioxides. <i>Physics and Chemistry of Minerals</i> , 2011 , 38, 387-395	1.6	26
42	first-principles investigation of hydrous defects and IR frequencies in forsterite: The case for Si vacancies. <i>American Mineralogist</i> , 2011 , 96, 1475-1479	2.9	36
41	Identification of post-pyrite phase transitions in SiO ₂ by a genetic algorithm. <i>Physical Review B</i> , 2011 , 83,	3.3	39
40	Ultrahigh-pressure phases of H ₂ O ice predicted using an adaptive genetic algorithm. <i>Physical Review B</i> , 2011 , 84,	3.3	64
39	9. Spin-State Crossover of Iron in Lower-Mantle Minerals: Results of DFT+U Investigations 2010 , 169-200		2
38	15. Computer Simulations on Phase Transitions in Ice 2010 , 315-336		
37	14. Multi-Mbar Phase Transitions in Minerals 2010 , 299-314		
36	Multi-Mbar Phase Transitions in Minerals. <i>Reviews in Mineralogy and Geochemistry</i> , 2010 , 71, 299-314	7.1	8
35	Body-centered tetragonal C4: a viable sp ³ carbon allotrope. <i>Physical Review Letters</i> , 2010 , 104, 125504	7.4	323
34	Correction to Pressure-volume-temperature relations in MgO: An ultrahigh pressure-temperature scale for planetary sciences applications \square <i>Journal of Geophysical Research</i> , 2010 , 115,		2
33	Fundamentals of elasticity of (Mg _{1-x} , Fe _x) ₂ SiO ₄ olivine. <i>Geophysical Research Letters</i> , 2010 , 37, n/a-n/a	4.9	16

32	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	7.1	30
31	Spin states and hyperfine interactions of iron in (Mg,Fe)SiO ₃ perovskite under pressure. <i>Earth and Planetary Science Letters</i> , 2010 , 294, 19-26	5.3	91
30	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	2.3	26
29	Computer Simulations on Phase Transitions in Ice. <i>Reviews in Mineralogy and Geochemistry</i> , 2010 , 71, 315-335	7.1	8
28	Order-disorder phase boundary between ice VII and VIII obtained by first principles. <i>Chemical Physics Letters</i> , 2010 , 499, 236-240	2.5	30
27	First-principles study for low-spin LaCoO ₃ with a structurally consistent Hubbard U. <i>Physical Review B</i> , 2009 , 79,	3.3	90
26	Lattice dynamics and thermal equation of state of platinum. <i>Physical Review B</i> , 2008 , 78,	3.3	33
25	Pressure-volume-temperature relations in MgO: An ultrahigh pressure-temperature scale for planetary sciences applications. <i>Journal of Geophysical Research</i> , 2008 , 113,		75
24	Spin transition in (Mg,Fe)SiO ₃ perovskite under pressure. <i>Earth and Planetary Science Letters</i> , 2008 , 276, 198-206	5.3	57
23	Prediction of an U2S3-type polymorph of Al ₂ O ₃ at 3.7 Mbar. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 6526-30	11.5	48
22	First principles investigation of the postspinel transition in Mg ₂ SiO ₄ . <i>Geophysical Research Letters</i> , 2007 , 34,	4.9	48
21	Composition controlled spin polarization in Co(1-x)Fe(x)S(2) alloys. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 315219	1.8	30
20	Thermodynamic Properties and Stability Field of MgSiO ₃ Post-Perovskite. <i>Geophysical Monograph Series</i> , 2007 , 79-97	1.1	1
19	Potential ultrahigh pressure polymorphs of ABX ₃ -type compounds. <i>Physical Review B</i> , 2006 , 74,	3.3	21
18	Dissociation of MgSiO ₃ in the cores of gas giants and terrestrial exoplanets. <i>Science</i> , 2006 , 311, 983-6	33.3	145
17	NaMgF ₃ : A low-pressure analog of MgSiO ₃ . <i>Geophysical Research Letters</i> , 2006 , 33,	4.9	35
16	Composition controlled spin polarization in Co _{1-x} Fe _x S ₂ : Electronic, magnetic, and thermodynamic properties. <i>Physical Review B</i> , 2006 , 73,	3.3	36
15	Electronic structure of Co _{1-x} Fe _x S ₂ . <i>Physica Status Solidi (B): Basic Research</i> , 2006 , 243, 2117-2121	1.3	20

14	Low-<high density transformations in ice. <i>Chemical Physics Letters</i> , 2005 , 405, 53-57	2.5	8
13	Co _{1-x} FexS ₂ : a tunable source of highly spin-polarized electrons. <i>Physical Review Letters</i> , 2005 , 94, 056602-4	7.4	68
12	Theoretical study of the isostructural transformation in ice VIII. <i>Physical Review B</i> , 2005 , 71,	3.3	20
11	Anomalous pressure-induced transition(s) in ice XI. <i>Physical Review Letters</i> , 2004 , 92, 105502	7.4	35
10	Amorphization in quenched ice VIII: A first-principles study. <i>Physical Review B</i> , 2004 , 69,	3.3	18
9	Energetics and structural stability of Cs ₃ C ₆₀ . <i>Solid State Communications</i> , 2004 , 130, 335-339	1.6	12
8	Elasticity of post-perovskite MgSiO ₃ . <i>Geophysical Research Letters</i> , 2004 , 31,	4.9	132
7	Phase transition in MgSiO ₃ perovskite in the earth's lower mantle. <i>Earth and Planetary Science Letters</i> , 2004 , 224, 241-248	5.3	495
6	Hierarchical assembly of nanostructured carbon foam. <i>Molecular Crystals and Liquid Crystals</i> , 2002 , 386, 189-195	0.5	8
5	Carbon foam: Spanning the phase space between graphite and diamond. <i>Physical Review B</i> , 2001 , 64,	3.3	70
4	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		
3	Electronic structure of the Ba ₄ C ₆₀ superconductor. <i>Physical Review B</i> , 2000 , 61, 14204-14208	3.3	13
2	Electronic structure of K ₃ Ba ₃ C ₆₀ and Rb ₃ Ba ₃ C ₆₀ superconductors. <i>Physical Review B</i> , 1999 , 60, 16186-16191	3.3	11
1	Electronic Configurations of Superheavy Elements. <i>Journal of the Physical Society of Japan</i> , 1996 , 65, 3175-3179	1.5	20