

# Koichiro Umemoto

## List of Publications by Citations

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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	Phase transition in MgSiO <sub>3</sub> perovskite in the earth's lower mantle. <i>Earth and Planetary Science Letters</i> , <b>2004</b> , 224, 241-248	5.3	495
66	Body-centered tetragonal C4: a viable sp <sup>3</sup> carbon allotrope. <i>Physical Review Letters</i> , <b>2010</b> , 104, 125504	7.4	323
65	Dissociation of MgSiO <sub>3</sub> in the cores of gas giants and terrestrial exoplanets. <i>Science</i> , <b>2006</b> , 311, 983-6	33.3	145
64	Elasticity of post-perovskite MgSiO <sub>3</sub> . <i>Geophysical Research Letters</i> , <b>2004</b> , 31,	4.9	132
63	Crystallization of silicon dioxide and compositional evolution of the Earth's core. <i>Nature</i> , <b>2017</b> , 543, 99-102	102.4	120
62	Spin states and hyperfine interactions of iron in (Mg,Fe)SiO <sub>3</sub> perovskite under pressure. <i>Earth and Planetary Science Letters</i> , <b>2010</b> , 294, 19-26	5.3	91
61	First-principles study for low-spin LaCoO <sub>3</sub> with a structurally consistent Hubbard U. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	90
60	Pressure-volume-temperature relations in MgO: An ultrahigh pressure-temperature scale for planetary sciences applications. <i>Journal of Geophysical Research</i> , <b>2008</b> , 113,		75
59	Carbon foam: Spanning the phase space between graphite and diamond. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	70
58	Co <sub>1-x</sub> Fe <sub>x</sub> S <sub>2</sub> : a tunable source of highly spin-polarized electrons. <i>Physical Review Letters</i> , <b>2005</b> , 94, 056602	7.4	68
57	Ultrahigh-pressure phases of H <sub>2</sub> O ice predicted using an adaptive genetic algorithm. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	64
56	Spin transition in (Mg,Fe)SiO <sub>3</sub> perovskite under pressure. <i>Earth and Planetary Science Letters</i> , <b>2008</b> , 276, 198-206	5.3	57
55	Two-stage dissociation in MgSiO <sub>3</sub> post-perovskite. <i>Earth and Planetary Science Letters</i> , <b>2011</b> , 311, 225-229	5.3	49
54	Prediction of an U <sub>2</sub> S <sub>3</sub> -type polymorph of Al <sub>2</sub> O <sub>3</sub> at 3.7 Mbar. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2008</b> , 105, 6526-30	11.5	48
53	First principles investigation of the postspinel transition in Mg <sub>2</sub> SiO <sub>4</sub> . <i>Geophysical Research Letters</i> , <b>2007</b> , 34,	4.9	48
52	Liquid iron-hydrogen alloys at outer core conditions by first-principles calculations. <i>Geophysical Research Letters</i> , <b>2015</b> , 42, 7513-7520	4.9	46
51	Identification of post-pyrite phase transitions in SiO <sub>2</sub> by a genetic algorithm. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	39

50	first-principles investigation of hydrous defects and IR frequencies in forsterite: The case for Si vacancies. <i>American Mineralogist</i> , <b>2011</b> , 96, 1475-1479	2.9	36
49	Composition controlled spin polarization in Co <sub>1-x</sub> Fe <sub>x</sub> S <sub>2</sub> : Electronic, magnetic, and thermodynamic properties. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	36
48	NaMgF <sub>3</sub> : A low-pressure analog of MgSiO <sub>3</sub> . <i>Geophysical Research Letters</i> , <b>2006</b> , 33,	4.9	35
47	Anomalous pressure-induced transition(s) in ice XI. <i>Physical Review Letters</i> , <b>2004</b> , 92, 105502	7.4	35
46	Liquid iron-sulfur alloys at outer core conditions by first-principles calculations. <i>Geophysical Research Letters</i> , <b>2014</b> , 41, 6712-6717	4.9	34
45	Lattice dynamics and thermal equation of state of platinum. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	33
44	Spin-State Crossover of Iron in Lower-Mantle Minerals: Results of DFT+U Investigations. <i>Reviews in Mineralogy and Geochemistry</i> , <b>2010</b> , 71, 169-199	7.1	30
43	Order-disorder phase boundary between ice VII and VIII obtained by first principles. <i>Chemical Physics Letters</i> , <b>2010</b> , 499, 236-240	2.5	30
42	Composition controlled spin polarization in Co(1-x)Fe(x)S(2) alloys. <i>Journal of Physics Condensed Matter</i> , <b>2007</b> , 19, 315219	1.8	30
41	Glycine Polymerization on Oxide Minerals. <i>Origins of Life and Evolution of Biospheres</i> , <b>2017</b> , 47, 123-143	1.5	29
40	Elasticity of diamond at high pressures and temperatures. <i>Applied Physics Letters</i> , <b>2012</b> , 101, 171902	3.4	27
39	Effect of the d electrons on phase transitions in transition-metal sesquioxides. <i>Physics and Chemistry of Minerals</i> , <b>2011</b> , 38, 387-395	1.6	26
38	Effect of site degeneracies on the spin crossovers in (Mg, Fe)SiO <sub>3</sub> perovskite. <i>Physics of the Earth and Planetary Interiors</i> , <b>2010</b> , 180, 209-214	2.3	26
37	Phase transitions in MgSiO <sub>3</sub> post-perovskite in super-Earth mantles. <i>Earth and Planetary Science Letters</i> , <b>2017</b> , 478, 40-45	5.3	24
36	The Hubbard U correction for iron-bearing minerals: A discussion based on (Mg,Fe)SiO <sub>3</sub> perovskite. <i>Physics of the Earth and Planetary Interiors</i> , <b>2011</b> , 185, 13-19	2.3	21
35	Potential ultrahigh pressure polymorphs of ABX <sub>3</sub> -type compounds. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	21
34	Electronic structure of Co <sub>1-x</sub> Fe <sub>x</sub> S <sub>2</sub> . <i>Physica Status Solidi (B): Basic Research</i> , <b>2006</b> , 243, 2117-2121	1.3	20
33	Theoretical study of the isostructural transformation in ice VIII. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	20

32	Electronic Configurations of Superheavy Elements. <i>Journal of the Physical Society of Japan</i> , <b>1996</b> , 65, 3175-3179	1.5	20
31	Amorphization in quenched ice VIII: A first-principles study. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	18
30	Chemical compositions of the outer core examined by first principles calculations. <i>Earth and Planetary Science Letters</i> , <b>2020</b> , 531, 116009	5.3	18
29	Nature of the Volume Isotope Effect in Ice. <i>Physical Review Letters</i> , <b>2015</b> , 115, 173005	7.4	17
28	Fundamentals of elasticity of (Mg <sub>1-x</sub> , Fe <sub>x</sub> ) <sub>2</sub> SiO <sub>4</sub> olivine. <i>Geophysical Research Letters</i> , <b>2010</b> , 37, n/a-n/a	4.9	16
27	Phase transition in SiC from zinc-blende to rock-salt structure and implications for carbon-rich extrasolar planets. <i>American Mineralogist</i> , <b>2017</b> , 102, 2230-2234	2.9	15
26	First-principles studies of spin-state crossovers of iron in perovskite. <i>European Journal of Mineralogy</i> , <b>2012</b> , 24, 851-862	2.2	14
25	Post-stishovite transition in hydrous aluminous SiO <sub>2</sub> . <i>Physics of the Earth and Planetary Interiors</i> , <b>2016</b> , 255, 18-26	2.3	14
24	Electronic structure of the Ba <sub>4</sub> C <sub>60</sub> superconductor. <i>Physical Review B</i> , <b>2000</b> , 61, 14204-14208	3.3	13
23	Ab initio study of water speciation in forsterite: Importance of the entropic effect. <i>American Mineralogist</i> , <b>2018</b> , 103, 692-699	2.9	13
22	Energetics and structural stability of Cs <sub>3</sub> C <sub>60</sub> . <i>Solid State Communications</i> , <b>2004</b> , 130, 335-339	1.6	12
21	Electronic structure of K <sub>3</sub> Ba <sub>3</sub> C <sub>60</sub> and Rb <sub>3</sub> Ba <sub>3</sub> C <sub>60</sub> superconductors. <i>Physical Review B</i> , <b>1999</b> , 60, 16186-16191	3.9	11
20	Mass-dependent dynamics of terrestrial exoplanets using ab initio mineral properties. <i>Icarus</i> , <b>2019</b> , 317, 412-426	3.8	11
19	Stability of fcc phase FeH to 137 GPa. <i>American Mineralogist</i> , <b>2020</b> , 105, 917-921	2.9	8
18	Multi-Mbar Phase Transitions in Minerals. <i>Reviews in Mineralogy and Geochemistry</i> , <b>2010</b> , 71, 299-314	7.1	8
17	Computer Simulations on Phase Transitions in Ice. <i>Reviews in Mineralogy and Geochemistry</i> , <b>2010</b> , 71, 315-335	7.1	8
16	Low-<high density transformations in ice. <i>Chemical Physics Letters</i> , <b>2005</b> , 405, 53-57	2.5	8
15	Hierarchical assembly of nanostructured carbon foam. <i>Molecular Crystals and Liquid Crystals</i> , <b>2002</b> , 386, 189-195	0.5	8

14	First principles study of volume isotope effects in ices VIII and X. <i>Japanese Journal of Applied Physics</i> , <b>2017</b> , 56, 05FA03	1.4	6
13	qha: A Python package for quasiharmonic free energy calculation for multi-configuration systems. <i>Computer Physics Communications</i> , <b>2019</b> , 237, 199-207	4.2	6
12	First-Principles Determination of the Dissociation Phase Boundary of Phase H MgSiO <sub>4</sub> H <sub>2</sub> . <i>Geophysical Research Letters</i> , <b>2019</b> , 46, 7333-7336	4.9	5
11	Ab initio exploration of post-PPV transitions in low-pressure analogs of MgSiO <sub>3</sub> . <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	3
10	9. Spin-State Crossover of Iron in Lower-Mantle Minerals: Results of DFT+U Investigations <b>2010</b> , 169-200		2
9	Correction to Pressure-volume-temperature relations in MgO: An ultrahigh pressure-temperature scale for planetary sciences applications <i>Journal of Geophysical Research</i> , <b>2010</b> , 115,		2
8	Two-stages Dissociation of NaMgF <sub>3</sub> Post-Perovskite: A Potential Low-Pressure Analog of MgSiO <sub>3</sub> at Multi-Mbar Pressures <b>2015</b> ,		1
7	Searching for high magnetization density in bulk Fe: the new metastable Fe $\beta$ phase. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 016001	1.8	1
6	Thermodynamic Properties and Stability Field of MgSiO <sub>3</sub> Post-Perovskite. <i>Geophysical Monograph Series</i> , <b>2007</b> , 79-97	1.1	1
5	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> , <b>2017</b> , 27, 205-212	0	
4	15. Computer Simulations on Phase Transitions in Ice <b>2010</b> , 315-336		
3	14. Multi-Mbar Phase Transitions in Minerals <b>2010</b> , 299-314		
2	Hybridization between K and C <sub>60</sub> Electronic States in Superconducting K <sub>3</sub> Ba <sub>3</sub> C <sub>60</sub> . <i>Molecular Crystals and Liquid Crystals</i> , <b>2000</b> , 340, 605-610		
1	Structural transition and re-emergence of iron's total electron spin in (Mg,Fe)O at ultrahigh pressure.. <i>Nature Communications</i> , <b>2022</b> , 13, 2780	17.4	