Renata M M Wentzcovitch

List of Publications by Year
in descending order

104 papers	23,844 citations	76326 40 h-index	30922 102 g-index
106 all docs	106 docs citations	106 times ranked	23517 citing authors

#	Article	IF	Citations
1	Two-step nucleation of the Earthâ€™s inner core. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	14
2	Thermodynamics of spin crossover in ferropericlase: an improved LDA + U_{sc} calculation. Electronic Structure, 2022, 4, 014008.	2.8	3
3	Structure and motifs of iron oxides from 1 to 3 TPa. Physical Review Materials, 2022, 6, .	2.4	1
4	Intermediate spin state and the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>B</mml:mi><mml:mn>1</mml:mn><mml:mtext>â†’</mml:mtext>â†’</mml:mrow></mml:math> transition in ferropericlase. Physical Review Research, 2022, 4, .	3.6	8
5	Ab initio investigation of H-bond disordering in Î´-AlOOH. Physical Review Research, 2022, 4, .	3.6	4
6	Ab initio anharmonic thermodynamic properties of cubic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ca</mml:mi><mml:mi>Si</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> perovskite. Physical Review B, 2021, 103, .	3.2	7
7	Ab initio lattice thermal conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mg</mml:mi><mml:mi>Si</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> across the perovskite-postperovskite phase transition. Physical Review B, 2021, 103, .	3.2	8
8	Thermodynamic properties of Îµ -Fe with thermal electronic excitation effects on vibrational spectra. Physical Review B, 2021, 103, .	3.2	11
9	Ab initio prediction of an order-disorder transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mg</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> : Implication for the nature of super-Earth's mantles. Physical Review Materials, 2021, 5, .	2.4	5
10	cij: A Python code for quasiharmonic thermoelasticity. Computer Physics Communications, 2021, 267, 108067.	7.5	13
11	Seismological expression of the iron spin crossover in ferropericlase in the Earthâ€™s lower mantle. Nature Communications, 2021, 12, 5905.	12.8	11
12	Unconventional iron-magnesium compounds at terapascal pressures. Physical Review B, 2021, 104, .	3.2	3
13	Thermal conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaSiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> perovskite at lower mantle conditions. Physical Review B, 2021, 104, .	3.2	2
14	Phonon dispersion throughout the iron spin crossover in ferropericlase. Physical Review B, 2020, 102, .	3.2	6
15	Toward an international practical pressure scale: A proposal for an IPPS ruby gauge (IPPS-Ruby2020). High Pressure Research, 2020, 40, 299-314.	1.2	143
16	Velocity and density characteristics of subducted oceanic crust and the origin of lower-mantle heterogeneities. Nature Communications, 2020, 11, 64.	12.8	30
17	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LDA</mml:mi><mml:mo>+</mml:mo><mml:msub> calculations of phase relations in FeO. Physical Review Materials, 2020, 4, .	2.4	14
18	Thermoelasticity of Ironâ€•and Aluminumâ€Bearing MgSiO₃ Postperovskite. Journal of Geophysical Research: Solid Earth, 2019, 124, 2417-2427.	3.4	5

#	Article	IF	Citations
19	qha: A Python package for quasiharmonic free energy calculation for multi-configuration systems. Computer Physics Communications, 2019, 237, 199-207.	7.5	21
20	Effects of Induced Stress on Seismic Waves: Validation Based on Ab Initio Calculations. Journal of Geophysical Research: Solid Earth, 2019, 124, 729-741.	3.4	8
21	Ab initio exploration of post-PPV transitions in low-pressure analogs of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MgSiO</mml:mi><mml:mn>3</mml:mn></mml:msub> Physical Review Materials, 2019, 3, .	2.4	10
22	An Extended Semianalytical Approach for Thermoelasticity of Monoclinic Crystals: Application to Diopside. Journal of Geophysical Research: Solid Earth, 2018, 123, 7629-7643.	3.4	18
23	Electronic structure of BaSnO3 investigated by high-energy-resolution electron energy-loss spectroscopy and ab initio calculations. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2018, 36, .	2.1	11
24	Persistence of strong silica-enriched domains in the Earthâ€™s lower mantle. Nature Geoscience, 2017, 10, 236-240.	12.9	138
25	Influence of the iron spin crossover in ferropericlase on the lower mantle geotherm. Geophysical Research Letters, 2017, 44, 4863-4871.	4.0	15
26	Bullen's Parameter as a Seismic Observable for Spin Crossovers in the Lower Mantle. Geophysical Research Letters, 2017, 44, 9314-9320.	4.0	1
27	Probing the Electronic Structure of BaSnO3 by EELS Analysis and ab initio Calculations. Microscopy and Microanalysis, 2017, 23, 1602-1603.	0.4	0
28	Phase transitions in MgSiO3 post-perovskite in super-Earth mantles. Earth and Planetary Science Letters, 2017, 478, 40-45.	4.4	45
29	Thermal conductivity from phonon quasiparticles with subminimal mean free path in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MgSiO</mml:mi><mml:mn>3</mml:mn></mml:msub> perovskite. Physical Review B, 2017, 96, .	3.2	15
30	Lattice Thermal Conductivity of MgSiO3 Perovskite from First Principles. Scientific Reports, 2017, 7, 5417.	3.3	23
31	Evolutionary optimization of PAW data-sets for accurate high pressure simulations. Journal of Computational Physics, 2017, 347, 39-55.	3.8	7
32	Composition versus temperature induced velocity heterogeneities in a pyrolitic lower mantle. Earth and Planetary Science Letters, 2017, 457, 359-365.	4.4	15
33	Spin crossover in (Mg,Fe3+)(Si,Fe3+)O3 bridgmanite: Effects of disorder, iron concentration, and temperature. Physics of the Earth and Planetary Interiors, 2016, 260, 53-61.	1.9	23
34	Thermoelasticity of Fe³⁺â€•and Alâ€bearing bridgmanite: Effects of iron spin crossover. Geophysical Research Letters, 2016, 43, 5661-5670.	4.0	43
35	A New Line Defect in NdTiO₃ Perovskite. Nano Letters, 2016, 16, 6816-6822.	9.1	18
36	Electronic Structure of New Line Defect in Strained NdTiCb on SrTiO3. Microscopy and Microanalysis, 2015, 21, 2073-2074.	0.4	0

#	Article	IF	Citations
37	Spin crossovers in iron-bearing MgSiO3 and MgGeO3: Their influence on the post-perovskite transition. Physics of the Earth and Planetary Interiors, 2015, 249, 11-17.	1.9	9
38	Accurate thermoelastic tensor and acoustic velocities of NaCl. AIP Advances, 2015, 5, 127222.	1.3	5
39	Thermoelasticity of Fe²⁺â€bearing bridgmanite. Geophysical Research Letters, 2015, 42, 1741-1749.	4.0	57
40	Two-stages Dissociation of NaMgF₃Post-Perovskite: A Potential Low-Pressure Analog of MgSiO₃at Multi-Mbar Pressures. , 2015, , .		1
41	Atomic and electronic structure of exfoliated black phosphorus. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2015, 33, .	2.1	73
42	Hybridab-initio/experimental high temperature equations of state: Application to the NaCl pressure scale. Journal of Applied Physics, 2015, 117, 215902.	2.5	8
43	First-principles elasticity of monocarboaluminate hydrates. American Mineralogist, 2014, 99, 1360-1368.	1.9	21
44	Dynamic stabilization of cubic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ca</mml:mi><mml:mi>Si</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>perovskite at high temperatures and pressures fromab initiomolecular dynamics. Physical Review B, 2014, 89, .	3.2	79
45	Phonon Quasiparticles and Anharmonic Free Energy in Complex Systems. Physical Review Letters, 2014, 112, 058501.	7.8	83
46	First-principles study of intermediate-spin ferrous iron in the Earth's lower mantle. Physical Review B, 2014, 90, .	3.2	30
47	Spin crossover in ferropericlase and velocity heterogeneities in the lower mantle. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10468-10472.	7.1	69
48	Elastic Anomalies in a Spin-Crossover System: Ferropericlase at Lower Mantle Conditions. Physical Review Letters, 2013, 110, 228501.	7.8	101
49	Elasticity of diamond at high pressures and temperatures. Applied Physics Letters, 2012, 101, .	3.3	37
50	Spin states and hyperfine interactions of iron incorporated in MgSiO3 post-perovskite. Earth and Planetary Science Letters, 2012, 331-332, 1-7.	4.4	36
51	Thermoelastic properties of ringwoodite (Fex,Mg1â^'x)2SiO4: Its relationship to the 520km seismic discontinuity. Earth and Planetary Science Letters, 2012, 351-352, 115-122.	4.4	34
52	Spin crossover of iron in aluminous MgSiO3 perovskite and post-perovskite. Earth and Planetary Science Letters, 2012, 359-360, 34-39.	4.4	56
53	Ferromagnetic insulating state in tensile-strained LaCoO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>thin films from LDA<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>+</mml:mo></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline">	3.2	66
54	Elastic Properties of Tricalcium Aluminate from Highâ€Pressure Experiments and Firstâ€Principles Calculations. Journal of the American Ceramic Society, 2012, 95, 2972-2978.	3.8	32

#	Article	IF	Citations
55	Quasiharmonic thermal elasticity of crystals: An analytical approach. Physical Review B, 2011, 83, .	3.2	62
56	Thermodynamic properties of MgSiO₃majorite and phase transitions near 660 km depth in MgSiO₃and Mg₂SiO₄: A first principles study. Journal of Geophysical Research, 2011, 116, .	3.3	41
57	Effect of the d electrons on phase transitions in transition-metal sesquioxides. Physics and Chemistry of Minerals, 2011, 38, 387-395.	0.8	31
58	Spin-State Crossover and Hyperfine Interactions of Ferric Iron in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>MgSiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Perovskite. Physical Review Letters, 2011, 106, 118501.	7.8	143
59	A first-principles investigation of hydrous defects and IR frequencies in forsterite: The case for Si vacancies. American Mineralogist, 2011, 96, 1475-1479.	1.9	53
60	Identification of post-pyrite phase transitions in SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>by a genetic algorithm. Physical Review B, 2011, 83, .	3.2	46
61	Ultrahigh-pressure phases of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O ice predicted using an adaptive genetic algorithm. Physical Review B, 2011, 84, .	3.2	72
62	First principles study of thermodynamics and phase transition in lowâ€pressure (P2₁/c) and highâ€pressure (C2/c) clinoenstatite MgSiO₃. Journal of Geophysical Research, 2010, 115, .	3.3	17
63	Spin states and hyperfine interactions of iron in (Mg,Fe)SiO3 perovskite under pressure. Earth and Planetary Science Letters, 2010, 294, 19-26.	4.4	102
64	Cobalt spin states and hyperfine interactions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaCoO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>LDA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>c Physical Review B, 2010, 82, .	3.2	44
65	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
66	First-principles study for low-spin<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaCoO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: a structurally consistent Hubbard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>. Physical Review B, 2009, 79, .	3.2	100
67	Lattice dynamics and thermal equation of state of platinum. Physical Review B, 2008, 78, .	3.2	47
68	Pressureâ€volumeâ€temperature relations in MgO: An ultrahigh pressureâ€temperature scale for planetary sciences applications. Journal of Geophysical Research, 2008, 113, .	3.3	84
69	Spin transition in (Mg,Fe)SiO3 perovskite under pressure. Earth and Planetary Science Letters, 2008, 276, 198-206.	4.4	65
70	Quasiharmonic elastic constants corrected for deviatoric thermal stresses. Physical Review B, 2008, 78, .	3.2	22
71	Vibrational properties of Â-AlOOH under pressure. American Mineralogist, 2008, 93, 477-482.	1.9	46
72	First-principles prediction of crystal structures at high temperatures using the quasiharmonic approximation. Physical Review B, 2007, 76, .	3.2	86

#	Article	IF	Citations
73	Thermodynamic Properties and Stability Field of MgSiO3 Post-Perovskite. Geophysical Monograph Series, 2007, , 79-97.	0.1	1
74	Vibrational and thermodynamic properties of forsterite at mantle conditions. Journal of Geophysical Research, 2007, 112, .	3.3	30
75	Electronic Spin Transition of Iron in the Earth's Deep Mantle. Eos, 2007, 88, 13.	0.1	13
76	First principles investigation of the postspinel transition in Mg2SiO4. Geophysical Research Letters, 2007, 34, .	4.0	55
77	Vibrational and thermodynamic properties of wadsleyite: A density functional study. Journal of Geophysical Research, 2007, 112, .	3.3	32
78	Dissociation of MgSiO3 in the Cores of Gas Giants and Terrestrial Exoplanets. Science, 2006, 311, 983-986.	12.6	166
79	Density functional study of vibrational and thermodynamic properties of ringwoodite. Journal of Geophysical Research, 2006, 111, n/a-n/a.	3.3	37
80	Spin Transition in MagnesiowÃ¼stite in Earthâ€™s Lower Mantle. Physical Review Letters, 2006, 96, 198501.	7.8	257
81	Pressure induced high spin to low spin transition in magnesiowÃ¼stite. Physica Status Solidi (B): Basic Research, 2006, 243, 2111-2116.	1.5	18
82	Theory of spintronic materials. Physica Status Solidi (B): Basic Research, 2006, 243, 2133-2150.	1.5	12
83	MgSiO3 postperovskite at D'' conditions. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 543-546.	7.1	180
84	Vibrational and thermodynamic properties of MgSiO3postperovskite. Journal of Geophysical Research, 2005, 110, .	3.3	105
85	Elasticity of post-perovskite MgSiO3. Geophysical Research Letters, 2004, 31, .	4.0	147
86	Phase transition in MgSiO3 perovskite in the earth's lower mantle. Earth and Planetary Science Letters, 2004, 224, 241-248.	4.4	571
87	Vibrational and quasiharmonic thermal properties of CaO under pressure. Physical Review B, 2003, 68, .	3.2	73
88	First-principles lattice dynamics and thermoelasticity of MgSiO3ilmenite at high pressure. Journal of Geophysical Research, 2002, 107, ECV 2-1-ECV 2-6.	3.3	23
89	High-pressure elastic properties of major materials of Earth's mantle from first principles. Reviews of Geophysics, 2001, 39, 507-534.	23.0	240
90	First principles thermoelasticity of MgSiO3-perovskite: Consequences for the inferred properties of the lower mantle. Geophysical Research Letters, 2001, 28, 2699-2702.	4.0	55

#	Article	IF	Citations
91	Ab initio study of MgSiO3 low-clinoenstatite at high pressure. American Mineralogist, 2001, 86, 762-766.	1.9	7
92	First principles description of the paramagnetic insulating state of chromia. Journal of Applied Physics, 2001, 89, 7201-7202.	2.5	4
93	Ab initio study of the elastic behavior of MgSiO3ilmenite at high pressure. Geophysical Research Letters, 1999, 26, 943-946.	4.0	29
94	High-pressure elasticity of alumina studied by first principles. American Mineralogist, 1999, 84, 1961-1966.	1.9	29
95	Normal and inverse ringwoodite at high pressures. American Mineralogist, 1999, 84, 288-293.	1.9	23
96	Optical Transitions in Ruby across the Corundum toRh2O3(II) Phase Transformation. Physical Review Letters, 1998, 81, 3267-3270.	7.8	36
97	A density functional study of the electronic structure of sodalite. Journal of Chemical Physics, 1998, 108, 8584-8588.	3.0	25
98	Ruby's Optical Transitions: Effects of Pressure-Induced Phase Transformation. Materials Research Society Symposia Proceedings, 1997, 499, 275.	0.1	1
99	Elastic constants and anisotropy of forsterite at high pressure. Geophysical Research Letters, 1997, 24, 1963-1966.	4.0	40
100	Calculated elastic constants and anisotropy of Mg2SiO4spinel at high pressure. Geophysical Research Letters, 1997, 24, 2841-2844.	4.0	80
101	High pressure studies of Mantle minerals by ab initio variable cell shape molecular dynamics. Molecular Engineering, 1996, 6, 39.	0.2	2
102	Ab initiomolecular dynamics with variable cell shape: Application toMgSiO3. Physical Review Letters, 1993, 70, 3947-3950.	7.8	301
103	Energy versus free-energy conservation in first-principles molecular dynamics. Physical Review B, 1992, 45, 11372-11374.	3.2	171
104	Invariant molecular-dynamics approach to structural phase transitions. Physical Review B, 1991, 44, 2358-2361.	3.2	321