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	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
2	Phase transition in MgSiO3 perovskite in the earth's lower mantle. Earth and Planetary Science Letters, 2004, 224, 241-248.	4.4	571
3	Invariant molecular-dynamics approach to structural phase transitions. Physical Review B, 1991, 44, 2358-2361.	3.2	321
4	Ab initiomolecular dynamics with variable cell shape: Application toMgSiO3. Physical Review Letters, 1993, 70, 3947-3950.	7.8	301
5	Spin Transition in MagnesiowÃ¼stite in Earthâ€™s Lower Mantle. Physical Review Letters, 2006, 96, 198501.	7.8	257
6	High-pressure elastic properties of major materials of Earth's mantle from first principles. Reviews of Geophysics, 2001, 39, 507-534.	23.0	240
7	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
8	Energy versus free-energy conservation in first-principles molecular dynamics. Physical Review B, 1992, 45, 11372-11374.	3.2	171
9	Dissociation of MgSiO3 in the Cores of Gas Giants and Terrestrial Exoplanets. Science, 2006, 311, 983-986.	12.6	166
10	Elasticity of post-perovskite MgSiO3. Geophysical Research Letters, 2004, 31, .	4.0	147
11	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
12	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
13	Persistence of strong silica-enriched domains in the Earthâ€™s lower mantle. Nature Geoscience, 2017, 10, 236-240.	12.9	138
14	Vibrational and thermodynamic properties of MgSiO3postperovskite. Journal of Geophysical Research, 2005, 110, .	3.3	105
15	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
16	Elastic Anomalies in a Spin-Crossover System: Ferropericlase at Lower Mantle Conditions. Physical Review Letters, 2013, 110, 228501.	7.8	101
17	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></m 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
18	First-principles prediction of crystal structures at high temperatures using the quasiharmonic approximation. Physical Review B, 2007, 76, .	3.2	86

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19	Pressureâ€volumeâ€temperature relations in MgO: An ultrahigh pressureâ€temperature scale for planetary sciences applications. Journal of Geophysical Research, 2008, 113, .	3.3	84
20	Phonon Quasiparticles and Anharmonic Free Energy in Complex Systems. Physical Review Letters, 2014, 112, 058501.	7.8	83
21	Calculated elastic constants and anisotropy of Mg2SiO4spinel at high pressure. Geophysical Research Letters, 1997, 24, 2841-2844.	4.0	80
22	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 from<i>ab initio</i>molecular dynamics. Physical Review B, 2014, 89, .	3.2	79
23	Vibrational and quasiharmonic thermal properties of CaO under pressure. Physical Review B, 2003, 68, .	3.2	73
24	Atomic and electronic structure of exfoliated black phosphorus. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2015, 33, .	2.1	73
25	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
26	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
27	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"><mml:mi>U</mml:mi></mml:math>	3.2	66
28	Spin transition in (Mg,Fe)SiO3 perovskite under pressure. Earth and Planetary Science Letters, 2008, 276, 198-206.	4.4	65
29	Quasiharmonic thermal elasticity of crystals: An analytical approach. Physical Review B, 2011, 83, .	3.2	62
30	Thermoelasticity of Fe²⁺â€bearing bridgmanite. Geophysical Research Letters, 2015, 42, 1741-1749.	4.0	57
31	Spin crossover of iron in aluminous MgSiO3 perovskite and post-perovskite. Earth and Planetary Science Letters, 2012, 359-360, 34-39.	4.4	56
32	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
33	First principles investigation of the postspinel transition in Mg2SiO4. Geophysical Research Letters, 2007, 34, .	4.0	55
34	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
35	Lattice dynamics and thermal equation of state of platinum. Physical Review B, 2008, 78, .	3.2	47
36	Vibrational properties of Â-AlOOH under pressure. American Mineralogist, 2008, 93, 477-482.	1.9	46

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37	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
38	Phase transitions in MgSiO3 post-perovskite in super-Earth mantles. Earth and Planetary Science Letters, 2017, 478, 40-45.	4.4	45
39	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></mm 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 Physical Review B, 2010, 82, .	3.2	44
40	Thermoelasticity of Fe³⁺â€•and Alâ€bearing bridgmanite: Effects of iron spin crossover. Geophysical Research Letters, 2016, 43, 5661-5670.	4.0	43
41	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
42	Elastic constants and anisotropy of forsterite at high pressure. Geophysical Research Letters, 1997, 24, 1963-1966.	4.0	40
43	Density functional study of vibrational and thermodynamic properties of ringwoodite. Journal of Geophysical Research, 2006, 111, n/a-n/a.	3.3	37
44	Elasticity of diamond at high pressures and temperatures. Applied Physics Letters, 2012, 101, .	3.3	37
45	Optical Transitions in Ruby across the Corundum toRh2O3(II) Phase Transformation. Physical Review Letters, 1998, 81, 3267-3270.	7.8	36
46	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
47	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
48	Vibrational and thermodynamic properties of wadsleyite: A density functional study. Journal of Geophysical Research, 2007, 112, .	3.3	32
49	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
50	Effect of the d electrons on phase transitions in transition-metal sesquioxides. Physics and Chemistry of Minerals, 2011, 38, 387-395.	0.8	31
51	Vibrational and thermodynamic properties of forsterite at mantle conditions. Journal of Geophysical Research, 2007, 112, .	3.3	30
52	First-principles study of intermediate-spin ferrous iron in the Earth's lower mantle. Physical Review B, 2014, 90, .	3.2	30
53	Velocity and density characteristics of subducted oceanic crust and the origin of lower-mantle heterogeneities. Nature Communications, 2020, 11, 64.	12.8	30
54	Ab initio study of the elastic behavior of MgSiO3ilmenite at high pressure. Geophysical Research Letters, 1999, 26, 943-946.	4.0	29

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55	High-pressure elasticity of alumina studied by first principles. American Mineralogist, 1999, 84, 1961-1966.	1.9	29
56	A density functional study of the electronic structure of sodalite. Journal of Chemical Physics, 1998, 108, 8584-8588.	3.0	25
57	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
58	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
59	Lattice Thermal Conductivity of MgSiO3 Perovskite from First Principles. Scientific Reports, 2017, 7, 5417.	3.3	23
60	Normal and inverse ringwoodite at high pressures. American Mineralogist, 1999, 84, 288-293.	1.9	23
61	Quasiharmonic elastic constants corrected for deviatoric thermal stresses. Physical Review B, 2008, 78, .	3.2	22
62	First-principles elasticity of monocarboaluminate hydrates. American Mineralogist, 2014, 99, 1360-1368.	1.9	21
63	qha: A Python package for quasiharmonic free energy calculation for multi-configuration systems. Computer Physics Communications, 2019, 237, 199-207.	7.5	21
64	Pressure induced high spin to low spin transition in magnesiowÃ¼stite. Physica Status Solidi (B): Basic Research, 2006, 243, 2111-2116.	1.5	18
65	A New Line Defect in NdTiO₃ Perovskite. Nano Letters, 2016, 16, 6816-6822.	9.1	18
66	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
67	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
68	Influence of the iron spin crossover in ferropericlase on the lower mantle geotherm. Geophysical Research Letters, 2017, 44, 4863-4871.	4.0	15
69	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
70	Composition versus temperature induced velocity heterogeneities in a pyrolitic lower mantle. Earth and Planetary Science Letters, 2017, 457, 359-365.	4.4	15
71	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LDA</mml:mi><mml:mo>+</mml:mo><mml:msub><mml calculations of phase relations in FeO. Physical Review Materials, 2020, 4, .	2.4	14
72	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

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73	Electronic Spin Transition of Iron in the Earth's Deep Mantle. Eos, 2007, 88, 13.	0.1	13
74	cij: A Python code for quasiharmonic thermoelasticity. Computer Physics Communications, 2021, 267, 108067.	7.5	13
75	Theory of spintronic materials. Physica Status Solidi (B): Basic Research, 2006, 243, 2133-2150.	1.5	12
76	Electronic structure of BaSnO3 investigated by high-energy-resolution electron energy-loss spectroscopy and <i>ab initio</i> calculations. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2018, 36, .	2.1	11
77	Thermodynamic properties of <i>Îµ</i> -Fe with thermal electronic excitation effects on vibrational spectra. Physical Review B, 2021, 103, .	3.2	11
78	Seismological expression of the iron spin crossover in ferropericlase in the Earthâ€™s lower mantle. Nature Communications, 2021, 12, 5905.	12.8	11
79	<i>Ab initio</i> 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
80	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
81	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></ perovskite at lower mantle conditions. Physical Review B, 2021, 104, .	3.2	9
82	Hybridab-initio/experimental high temperature equations of state: Application to the NaCl pressure scale. Journal of Applied Physics, 2015, 117, 215902.	2.5	8
83	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
84	<i>Ab initio</i> 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:m 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
85	Ab initio study of MgSiO3 low-clinoenstatite at high pressure. American Mineralogist, 2001, 86, 762-766.	1.9	7
86	Evolutionary optimization of PAW data-sets for accurate high pressure simulations. Journal of Computational Physics, 2017, 347, 39-55.	3.8	7
87	<i>Ab initio</i> 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 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
88	Phonon dispersion throughout the iron spin crossover in ferropericlase. Physical Review B, 2020, 102, .	3.2	6
89	Accurate thermoelastic tensor and acoustic velocities of NaCl. AIP Advances, 2015, 5, 127222.	1.3	5
90	Thermoelasticity of Ironâ€•and Aluminumâ€Bearing MgSiO₃ Postperovskite. Journal of Geophysical Research: Solid Earth, 2019, 124, 2417-2427.	3.4	5

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91	<i>Ab initio</i> 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></m 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
92	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`'</mm transition in ferropericlase. Physical Review Research, 2022, 4, .	3.6	5
93	First principles description of the paramagnetic insulating state of chromia. Journal of Applied Physics, 2001, 89, 7201-7202.	2.5	4
94	<i>Ab initio</i> investigation of H-bond disordering in Î´-AlOOH. Physical Review Research, 2022, 4, .	3.6	4
95	Unconventional iron-magnesium compounds at terapascal pressures. Physical Review B, 2021, 104, .	3.2	3
96	Thermodynamics of spin crossover in ferropericlase: an improved LDA + U_{sc} calculation. Electronic Structure, 2022, 4, 014008.	2.8	3
97	High pressure studies of Mantle minerals by ab initio variable cell shape molecular dynamics. Molecular Engineering, 1996, 6, 39.	0.2	2
98	Ruby's Optical Transitions: Effects of Pressure-Induced Phase Transformation. Materials Research Society Symposia Proceedings, 1997, 499, 275.	0.1	1
99	Thermodynamic Properties and Stability Field of MgSiO3 Post-Perovskite. Geophysical Monograph Series, 2007, , 79-97.	0.1	1
100	Two-stages Dissociation of NaMgF₃Post-Perovskite: A Potential Low-Pressure Analog of MgSiO₃at Multi-Mbar Pressures. , 2015, , .		1
101	Bullen's Parameter as a Seismic Observable for Spin Crossovers in the Lower Mantle. Geophysical Research Letters, 2017, 44, 9314-9320.	4.0	1
102	Structure and motifs of iron oxides from 1 to 3 TPa. Physical Review Materials, 2022, 6, .	2.4	1
103	Electronic Structure of New Line Defect in Strained NdTiCb on SrTiO3. Microscopy and Microanalysis, 2015, 21, 2073-2074.	0.4	0
104	Probing the Electronic Structure of BaSnO3 by EELS Analysis and ab initio Calculations. Microscopy and Microanalysis, 2017, 23, 1602-1603.	0.4	0