Andrew M Walker

List of Publications by Year
in descending order

66 papers	1,674 citations	257450 24 h-index	302126 39 g-index
78 all docs	78 docs citations	78 times ranked	1931 citing authors

#	Article	IF	Citations
1	Flexibility in a Metalâ€"Organic Framework Material Controlled by Weak Dispersion Forces: The Bistability of MILâ€53(Al). Angewandte Chemie - International Edition, 2010, 49, 7501-7503.	13.8	158
2	MSATâ€"A new toolkit for the analysis of elastic and seismic anisotropy. Computers and Geosciences, 2012, 49, 81-90.	4.2	128
3	Titanium substitution mechanisms in forsterite. Chemical Geology, 2007, 242, 176-186.	3.3	83
4	Three water sites in upper mantle olivine and the role of titanium in the water weakening mechanism. Journal of Geophysical Research, 2007, 112, .	3.3	74
5	Ti site occupancy in zircon. Geochimica Et Cosmochimica Acta, 2011, 75, 905-921.	3.9	72
6	An Ã¥ngstrÃ¶m-sized window on the origin of water in the inner solar system: Atomistic simulation of adsorption of water on olivine. Journal of Crystal Growth, 2006, 294, 83-95.	1.5	63
7	A computational study of oxygen diffusion in olivine. Physics and Chemistry of Minerals, 2003, 30, 536-545.	0.8	58
8	Predicting the structure of screw dislocations in nanoporous materials. Nature Materials, 2004, 3, 715-720.	27.5	56
9	Elastic anisotropy of Dâ€³ predicted from global models of mantle flow. Geochemistry, Geophysics, Geosystems, 2011, 12, n/a-n/a.	2.5	56
10	Variation of thermal conductivity and heat flux at the Earth's core mantle boundary. Earth and Planetary Science Letters, 2014, 390, 175-185.	4.4	48
11	Computer modelling of the energies and vibrational properties of hydroxyl groups in - and -Mg2SiO4. European Journal of Mineralogy, 2006, 18, 529-543.	1.3	44
12	Defects and dislocations in MgO: atomic scale models of impurity segregation and fast pipe diffusion. Journal of Materials Chemistry, 2010, 20, 10445.	6.7	40
13	Strong inheritance of texture between perovskite and post-perovskite in the Dâ€²â€² layer. Nature Geoscience, 2013, 6, 575-578.	12.9	40
14	Atomic scale modelling of the cores of dislocations in complex materials part 2: applications. Physical Chemistry Chemical Physics, 2005, 7, 3235.	2.8	39
15	A computational study of magnesium point defects and diffusion in forsterite. Physics of the Earth and Planetary Interiors, 2009, 172, 20-27.	1.9	39
16	The NiSi melting curve to 70GPa. Physics of the Earth and Planetary Interiors, 2014, 233, 13-23.	1.9	36
17	Development of texture and seismic anisotropy during the onset of subduction. Geochemistry, Geophysics, Geosystems, 2014, 15, 192-212.	2.5	36
18	Substitution of Ti3+ and Ti4+ in hibonite (CaAl12O19). American Mineralogist, 2014, 99, 1369-1382.	1.9	35

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19	On the increase in thermal diffusivity caused by the perovskite to post-perovskite phase transition and its implications for mantle dynamics. Earth and Planetary Science Letters, 2012, 319-320, 96-103.	4.4	33
20	Evaluating post-perovskite as a cause of Dâ€²â€² anisotropy in regions of palaeosubduction. Geophysical Journal International, 2013, 192, 1085-1090.	2.4	31
21	The effect of pressure on the elastic properties and seismic anisotropy of diopside and jadeite from atomic scale simulation. Physics of the Earth and Planetary Interiors, 2012, 192-193, 81-89.	1.9	28
22	Atomic scale modelling of the cores of dislocations in complex materials part 1: methodology. Physical Chemistry Chemical Physics, 2005, 7, 3227.	2.8	26
23	Atomic-scale models of dislocation cores in minerals: progress and prospects. Mineralogical Magazine, 2010, 74, 381-413.	1.4	26
24	Seismic evidence for flow in the hydrated mantle wedge of the Ryukyu subduction zone. Scientific Reports, 2016, 6, 29981.	3.3	24
25	The origin of the compressibility anomaly in amorphous silica: a molecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 275210.	1.8	22
26	The compressibility and high pressure structure of diopside from first principles simulation. Physics and Chemistry of Minerals, 2008, 35, 359-366.	0.8	22
27	Evidence from numerical modelling for 3D spreading of [001] screw dislocations in Mg₂SiO₄forsterite. Philosophical Magazine, 2008, 88, 2477-2485.	1.6	22
28	Bulk and Surface Simulation Studies of La1-xCaxMnO3. Chemistry of Materials, 2006, 18, 1552-1560.	6.7	21
29	Melt organisation and strain partitioning in the lower crust. Journal of Structural Geology, 2018, 113, 188-199.	2.3	21
30	A computational study of order-disorder phenomena in Mg2TiO4 spinel (qandilite). American Mineralogist, 2008, 93, 1363-1372.	1.9	16
31	Comment upon the screw dislocation structure on HKUST-1 {111} surfaces. CrystEngComm, 2008, 10, 790.	2.6	16
32	From data to analysis: linking NWChem and Avogadro with the syntax and semantics of Chemical Markup Language. Journal of Cheminformatics, 2013, 5, 25.	6.1	16
33	Thermoelastic properties of magnesiowÃ¼stite, (Mg_{1âˆ’<i>x</i>}Fe_{<i>x</i>})O: determination of the Andersonâ€“GrÃ¼neisen parameter by time-of-flight neutron powder diffraction at simultaneous high pressures and temperatures. Journal of Applied Crystallography, 2008, 41, 886-896.	4.5	15
34	Integrating computing, data and collaboration grids: the RMCS tool. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 1047-1050.	3.4	14
35	Thermal diffusivity of MORB-composition rocks to 15ÂGPa: implications for triggering of deep seismicity. High Pressure Research, 2010, 30, 406-414.	1.2	14
36	Peierls-Nabarro modeling of dislocations in UO 2. Journal of Nuclear Materials, 2017, 495, 202-210.	2.7	12

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37	Evolution of a shear zone before, during and after melting. Journal of the Geological Society, 2020, 177, 738-751.	2.1	12
38	The effect of pressure on thermal diffusivity in pyroxenes. Mineralogical Magazine, 2011, 75, 2597-2610.	1.4	11
39	The limitations of hibonite as a single-mineral oxybarometer for early solar system processes. Chemical Geology, 2017, 466, 32-40.	3.3	11
40	The anisotropic signal of topotaxy during phase transitions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si23.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mtext>D</mml:mtext></mml:mrow><mml:mrow><mml:mo>â€³</mml Physics of the Earth and Planetary Interiors, 2018, 276, 159-171.	1.9	11
41	Job submission to grid computing environments. Concurrency Computation Practice and Experience, 2008, 20, 1329-1340.	2.2	10
42	Molecular dynamics in a grid computing environment: experiences using DL_POLY_3 within theeMinerals escience project. Molecular Simulation, 2006, 32, 945-952.	2.0	9
43	Lessons in scientific data interoperability: XML and the <i>e</i> Minerals project. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 1041-1046.	3.4	9
44	Simulation of screw dislocations in wadsleyite. Physics and Chemistry of Minerals, 2010, 37, 301-310.	0.8	9
45	The effect of cation order on the elasticity of omphacite from atomistic calculations. Physics and Chemistry of Minerals, 2015, 42, 677-691.	0.8	9
46	Modeling the impact of melt on seismic properties during mountain building. Geochemistry, Geophysics, Geosystems, 2017, 18, 1090-1110.	2.5	9
47	Explaining the dependence of M-site diffusion in forsterite on silica activity: a density functional theory approach. Physics and Chemistry of Minerals, 2020, 47, 55.	0.8	9
48	eScience for molecular-scale simulations and the <i>e</i> Minerals project. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 967-985.	3.4	8
49	The phase diagram of NiSi under the conditions of small planetary interiors. Physics of the Earth and Planetary Interiors, 2016, 261, 196-206.	1.9	8
50	In-situ measurement of texture development rate in CaIrO3 post-perovskite. Physics of the Earth and Planetary Interiors, 2016, 257, 91-104.	1.9	8
51	New software for finding transition states by probing accessible, or ergodic, regions. Molecular Simulation, 2007, 33, 1229-1231.	2.0	7
52	Controls on the distribution of hydrous defects in forsterite from a thermodynamic model. Physics and Chemistry of Minerals, 2022, 49, 1.	0.8	6
53	The mechanism of Mg diffusion in forsterite and the controls on its anisotropy. Physics of the Earth and Planetary Interiors, 2021, 321, 106805.	1.9	5
54	Analytical parametrization of self-consistent polycrystal mechanics: Fast calculation of upper mantle anisotropy. Geophysical Journal International, 2015, 203, 334-350.	2.4	4

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55	Ab initio crystal structure and elasticity of tuite, Î³-Ca3(PO4)2, with implications for trace element partitioning in the lower mantle. Contributions To Mineralogy and Petrology, 2017, 172, 1.	3.1	4
56	Probing the nucleation of iron in Earth's core using molecular dynamics simulations of supercooled liquids. Physical Review B, 2021, 103, .	3.2	4
57	The Ti environment in natural hibonite: XANES spectroscopy and computer modelling. Journal of Physics: Conference Series, 2016, 712, 012089.	0.4	3
58	Lubrication of dislocation glide in MgO by hydrous defects. Physics and Chemistry of Minerals, 2018, 45, 713-726.	0.8	3
59	Lubrication of dislocation glide in forsterite by Mg vacancies: Insights from Peierls-Nabarro modeling. Physics of the Earth and Planetary Interiors, 2019, 287, 1-9.	1.9	3
60	Integrating Data Management and Collaborative Sharing with Computational Science Research Processes. Advances in Computer and Electrical Engineering Book Series, 2012, , 506-538.	0.3	3
61	Interactions between bare and protonated Mg vacancies and dislocation cores in MgO. Physics and Chemistry of Minerals, 2019, 46, 471-485.	0.8	2
62	The Conductive Cooling of Planetesimals With Temperatureâ€Dependent Properties. Journal of Geophysical Research E: Planets, 2021, 126, e2020JE006726.	3.6	2
63	Information Delivery in Computational Mineral Science: The eMinerals Data Handling System. , 2006, , .		1
64	Thermoelastic properties of MgSiO3-majorite at high temperatures and pressures: A first principles study. Physics of the Earth and Planetary Interiors, 2020, 303, 106491.	1.9	1
65	Large Scale Atomistic Simulation with Electrostatics: The Case of Cation Impurity Segregation Along an Edge Dislocation Line. , 2010, , .		0
66	Limits of the power law. Nature, 2012, 481, 153-154.	27.8	0