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	Controls on the distribution of hydrous defects in forsterite from a thermodynamic model. Physics and Chemistry of Minerals, 2022, 49, 1.	0.8	6
2	The Conductive Cooling of Planetesimals With Temperatureâ€Dependent Properties. Journal of Geophysical Research E: Planets, 2021, 126, e2020JE006726.	3.6	2
3	Probing the nucleation of iron in Earth's core using molecular dynamics simulations of supercooled liquids. Physical Review B, 2021, 103, .	3.2	4
4	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
5	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
6	Evolution of a shear zone before, during and after melting. Journal of the Geological Society, 2020, 177, 738-751.	2.1	12
7	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
8	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
9	Interactions between bare and protonated Mg vacancies and dislocation cores in MgO. Physics and Chemistry of Minerals, 2019, 46, 471-485.	0.8	2
10	Lubrication of dislocation glide in MgO by hydrous defects. Physics and Chemistry of Minerals, 2018, 45, 713-726.	0.8	3
11	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:mo></mml:mrow> Physics of the Earth and Planetary Interiors, 2018, 276, 159-171.	1.9	11
12	Melt organisation and strain partitioning in the lower crust. Journal of Structural Geology, 2018, 113, 188-199.	2.3	21
13	Modeling the impact of melt on seismic properties during mountain building. Geochemistry, Geophysics, Geosystems, 2017, 18, 1090-1110.	2.5	9
14	The limitations of hibonite as a single-mineral oxybarometer for early solar system processes. Chemical Geology, 2017, 466, 32-40.	3.3	11
15	Peierls-Nabarro modeling of dislocations in UO 2. Journal of Nuclear Materials, 2017, 495, 202-210.	2.7	12
16	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
17	Seismic evidence for flow in the hydrated mantle wedge of the Ryukyu subduction zone. Scientific Reports, 2016, 6, 29981.	3.3	24
18	The Ti environment in natural hibonite: XANES spectroscopy and computer modelling. Journal of Physics: Conference Series, 2016, 712, 012089.	0.4	3

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19	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
20	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
21	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
22	Analytical parametrization of self-consistent polycrystal mechanics: Fast calculation of upper mantle anisotropy. Geophysical Journal International, 2015, 203, 334-350.	2.4	4
23	Substitution of Ti3+ and Ti4+ in hibonite (CaAl12O19). American Mineralogist, 2014, 99, 1369-1382.	1.9	35
24	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
25	The NiSi melting curve to 70GPa. Physics of the Earth and Planetary Interiors, 2014, 233, 13-23.	1.9	36
26	Development of texture and seismic anisotropy during the onset of subduction. Geochemistry, Geophysics, Geosystems, 2014, 15, 192-212.	2.5	36
27	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
28	Strong inheritance of texture between perovskite and post-perovskite in the Dâ€²â€² layer. Nature Geoscience, 2013, 6, 575-578.	12.9	40
29	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
30	Limits of the power law. Nature, 2012, 481, 153-154.	27.8	0
31	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
32	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
33	MSATâ€"A new toolkit for the analysis of elastic and seismic anisotropy. Computers and Geosciences, 2012, 49, 81-90.	4.2	128
34	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
35	Elastic anisotropy of Dâ€³ predicted from global models of mantle flow. Geochemistry, Geophysics, Geosystems, 2011, 12, n/a-n/a.	2.5	56
36	Ti site occupancy in zircon. Geochimica Et Cosmochimica Acta, 2011, 75, 905-921.	3.9	72

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37	The effect of pressure on thermal diffusivity in pyroxenes. Mineralogical Magazine, 2011, 75, 2597-2610.	1.4	11
38	Simulation of screw dislocations in wadsleyite. Physics and Chemistry of Minerals, 2010, 37, 301-310.	0.8	9
39	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
40	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
41	Atomic-scale models of dislocation cores in minerals: progress and prospects. Mineralogical Magazine, 2010, 74, 381-413.	1.4	26
42	Thermal diffusivity of MORB-composition rocks to 15ÂGPa: implications for triggering of deep seismicity. High Pressure Research, 2010, 30, 406-414.	1.2	14
43	Large Scale Atomistic Simulation with Electrostatics: The Case of Cation Impurity Segregation Along an Edge Dislocation Line. , 2010, , .		0
44	Lessons in scientific data interoperability: XML and the e Minerals project. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 1041-1046.	3.4	9
45	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
46	eScience for molecular-scale simulations and the e Minerals project. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 967-985.	3.4	8
47	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
48	The compressibility and high pressure structure of diopside from first principles simulation. Physics and Chemistry of Minerals, 2008, 35, 359-366.	0.8	22
49	Thermoelastic properties of magnesiowÃ¼stite, (Mg_{1â^'x}Fe_x)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
50	Job submission to grid computing environments. Concurrency Computation Practice and Experience, 2008, 20, 1329-1340.	2.2	10
51	A computational study of order-disorder phenomena in Mg2TiO4 spinel (qandilite). American Mineralogist, 2008, 93, 1363-1372.	1.9	16
52	Comment upon the screw dislocation structure on HKUST-1 {111} surfaces. CrystEngComm, 2008, 10, 790.	2.6	16
53	Evidence from numerical modelling for 3D spreading of [001] screw dislocations in Mg₂SiO₄forsterite. Philosophical Magazine, 2008, 88, 2477-2485.	1.6	22
54	Titanium substitution mechanisms in forsterite. Chemical Geology, 2007, 242, 176-186.	3.3	83

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55	The origin of the compressibility anomaly in amorphous silica: a molecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 275210.	1.8	22
56	New software for finding transition states by probing accessible, or ergodic, regions. Molecular Simulation, 2007, 33, 1229-1231.	2.0	7
57	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
58	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
59	Information Delivery in Computational Mineral Science: The eMinerals Data Handling System. , 2006, , .		1
60	Bulk and Surface Simulation Studies of La1-xCaxMnO3. Chemistry of Materials, 2006, 18, 1552-1560.	6.7	21
61	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
62	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
63	Atomic scale modelling of the cores of dislocations in complex materials part 2: applications. Physical Chemistry Chemical Physics, 2005, 7, 3235.	2.8	39
64	Atomic scale modelling of the cores of dislocations in complex materials part 1: methodology. Physical Chemistry Chemical Physics, 2005, 7, 3227.	2.8	26
65	Predicting the structure of screw dislocations in nanoporous materials. Nature Materials, 2004, 3, 715-720.	27.5	56
66	A computational study of oxygen diffusion in olivine. Physics and Chemistry of Minerals, 2003, 30, 536-545.	0.8	58