## Stephen Stackhouse

List of Publications by Year in descending order

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#	Article	lF	CITATIONS
1	Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. Nature, 2005, 438, 1004-1007.	13.7	188
2	Caesium incorporation and retention in illite interlayers. Applied Clay Science, 2015, 108, 128-134.	2.6	155
3	The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO3. Earth and Planetary Science Letters, 2005, 230, 1-10.	1.8	137
4	Thermal Conductivity of Periclase (MgO) from First Principles. Physical Review Letters, 2010, 104, 208501.	2.9	125
5	On the application of computer simulation techniques to anionic and cationic clays: A materials chemistry perspective. Journal of Materials Chemistry, 2006, 16, 708-723.	6.7	124
6	Electronic spin transitions in iron-bearing MgSiO3 perovskite. Earth and Planetary Science Letters, 2007, 253, 282-290.	1.8	93
7	Plane-Wave Density Functional Theoretic Study of Formation of Clay-Polymer Nanocomposite Materials by Self-Catalyzed in Situ Intercalative Polymerization. Journal of the American Chemical Society, 2001, 123, 11764-11774.	6.6	79
8	A New Design Strategy for Molecular Recognition in Heterogeneous Systems:Â A Universal Crystal-Face Growth Inhibitor for Barium Sulfate. Journal of the American Chemical Society, 2000, 122, 11557-11558.	6.6	67
9	A Density Functional Theory Study of Catalytictrans-Esterification bytert-Butoxide MgAl Anionic Clays. Journal of Physical Chemistry B, 2003, 107, 3476-3485.	1.2	60
10	Elastic anisotropy of FeSiO3end-members of the perovskite and post-perovskite phases. Geophysical Research Letters, 2006, 33, n/a-n/a.	1.5	59
11	Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO3post-perovskite. Geophysical Research Letters, 2006, 33, .	1.5	50
12	Variation of thermal conductivity and heat flux at the Earth's core mantle boundary. Earth and Planetary Science Letters, 2014, 390, 175-185.	1.8	48
13	Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. Geophysical Research Letters, 2005, 32, .	1.5	47
14	Simulation of hydrated Li+-, Na+- and K+-montmorillonite/polymer nanocomposites using large-scale molecular dynamics. Chemical Physics Letters, 2004, 389, 261-267.	1.2	45
15	Density-Functional-Theory-Based Study of the Dehydroxylation Behavior of Aluminous Dioctahedral 2:1 Layer-Type Clay Minerals. Journal of Physical Chemistry B, 2004, 108, 9685-9694.	1.2	45
16	First-principles calculations of the lattice thermal conductivity of the lower mantle. Earth and Planetary Science Letters, 2015, 427, 11-17.	1.8	44
17	Elasticity of (Mg, Fe)(Si, Al)O3-perovskite at high pressure. Earth and Planetary Science Letters, 2005, 240, 529-536.	1.8	42
18	High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al2O3. Geophysical Research Letters, 2005, 32, .	1.5	37

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#	ARTICLE	IF	CITATIONS
19	Study of Thermally Treated Lithium Montmorillonite by Ab Initio Methods. Journal of Physical Chemistry B, 2002, 106, 12470-12477.	1.2	35
20	Determination of the high-pressure properties of fayalite from first-principles calculations. Earth and Planetary Science Letters, 2010, 289, 449-456.	1.8	33
21	The enigma of post-perovskite anisotropy: deformation versus transformation textures. Physics and Chemistry of Minerals, 2011, 38, 665-678.	0.3	33
22	High-pressure, temperature elasticity of Fe- and Al-bearing MgSiO3: Implications for the Earth's lower mantle. Earth and Planetary Science Letters, 2016, 434, 264-273.	1.8	32
23	Configuring pnicogen rings in skutterudites for low phonon conductivity. Physical Review B, 2012, 86,	1.1	30
24	Shear-induced material transfer across the core-mantle boundary aided by the post-perovskite phase transition. Earth, Planets and Space, 2005, 57, 459-464.	0.9	24
25	The rational design, synthesis and demonstration of the recognition and binding of a diaza-dioxa-12-crown-4 diphosphonate macrocycle to all crystal growth faces of barium sulfate. Perkin Transactions II RSC, 2002, , 1238-1245.	1.1	19
26	Methodology for determining the electronic thermal conductivity of metals via direct nonequilibrium <i>ab initio</i> molecular dynamics. Physical Review B, 2016, 94, .	1.1	17
27	Elastic properties of the post-perovskite phase of Fe2O3 and implications for ultra-low velocity zones. Physics of the Earth and Planetary Interiors, 2008, 170, 260-266.	0.7	15
28	The high-temperature elasticity of MgSiO3 post-perovskite. Geophysical Monograph Series, 2007, , 99-113.	0.1	14
29	Equations of state and stability of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"&gt;<mml:msub><mml:mi mathvariant="normal"&gt;MgSiO<mml:mn>3</mml:mn></mml:mi </mml:msub>perovskite and post-perovskite phases from quantum Monte Carlo simulations. Physical Review B, 2014, 90, .</mml:math 	1.1	11
30	Frontispiece: Ion Association in Lanthanide Chloride Solutions. Chemistry - A European Journal, 2019, 25, .	1.7	9
31	The spin deep within. Nature Geoscience, 2008, 1, 648-650.	5.4	7
32	Ion Association in Lanthanide Chloride Solutions. Chemistry - A European Journal, 2019, 25, 8725-8740.	1.7	5
33	The Rational Design, Synthesis and Demonstration of the Recognition and Binding of a Diazaâ€Dioxaâ€12â€crownâ€4 Diphosphonate Macrocycle (I) to All Crystal Growth Faces of Barium Sulfate ChemInform, 2002, 33, 173-173.	0.1	0
34	Gaining Insight into the Structure and Dynamics of Clay–Polymer Nanocomposite Systems Through Computer Simulation. , 2008, , 175-203.		0