Stephen Stackhouse

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

1,542 23 32 35 h-index g-index citations papers 6.8 1,627 35 4.3 L-index avg, IF ext. papers ext. citations

#	Paper	IF	Citations
32	Ion Association in Lanthanide Chloride Solutions. <i>Chemistry - A European Journal</i> , 2019 , 25, 8725-8740	4.8	2
31	Frontispiece: Ion Association in Lanthanide Chloride Solutions. <i>Chemistry - A European Journal</i> , 2019 , 25,	4.8	8
30	Methodology for determining the electronic thermal conductivity of metals via direct nonequilibrium ab initio molecular dynamics. <i>Physical Review B</i> , 2016 , 94,	3.3	16
29	High-pressure, temperature elasticity of Fe- and Al-bearing MgSiO3: Implications for the Earth lower mantle. <i>Earth and Planetary Science Letters</i> , 2016 , 434, 264-273	5.3	28
28	First-principles calculations of the lattice thermal conductivity of the lower mantle. <i>Earth and Planetary Science Letters</i> , 2015 , 427, 11-17	5.3	30
27	Caesium incorporation and retention in illite interlayers. <i>Applied Clay Science</i> , 2015 , 108, 128-134	5.2	124
26	Variation of thermal conductivity and heat flux at the Earth's core mantle boundary. <i>Earth and Planetary Science Letters</i> , 2014 , 390, 175-185	5.3	37
25	Equations of state and stability of MgSiO3 perovskite and post-perovskite phases from quantum Monte Carlo simulations. <i>Physical Review B</i> , 2014 , 90,	3.3	9
24	Configuring pnicogen rings in skutterudites for low phonon conductivity. <i>Physical Review B</i> , 2012 , 86,	3.3	28
23	The enigma of post-perovskite anisotropy: deformation versus transformation textures. <i>Physics and Chemistry of Minerals</i> , 2011 , 38, 665-678	1.6	31
22	Thermal conductivity of periclase (MgO) from first principles. <i>Physical Review Letters</i> , 2010 , 104, 20850	1 _{7.4}	101
21	Determination of the high-pressure properties of fayalite from first-principles calculations. <i>Earth and Planetary Science Letters</i> , 2010 , 289, 449-456	5.3	31
20	Elastic properties of the post-perovskite phase of Fe2O3 and implications for ultra-low velocity zones. <i>Physics of the Earth and Planetary Interiors</i> , 2008 , 170, 260-266	2.3	15
19	Gaining Insight into the Structure and Dynamics of ClayPolymer Nanocomposite Systems Through Computer Simulation 2008 , 175-203		
18	Electronic spin transitions in iron-bearing MgSiO3 perovskite. <i>Earth and Planetary Science Letters</i> , 2007 , 253, 282-290	5.3	89
17	The High-Temperature Elasticity of MgSiO3 Post-Perovskite. <i>Geophysical Monograph Series</i> , 2007 , 99-1	131.1	11
16	On the application of computer simulation techniques to anionic and cationic clays: A materials chemistry perspective. <i>Journal of Materials Chemistry</i> , 2006 , 16, 708-723		119

LIST OF PUBLICATIONS

Elastic anisotropy of FeSiO3 end-members of the perovskite and post-perovskite phases. <i>Geophysical Research Letters</i> , 2006 , 33, n/a-n/a	4.9	55
Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO3 post-perovskite. <i>Geophysical Research Letters</i> , 2006 , 33,	4.9	44
Shear-induced material transfer across the core-mantle boundary aided by the post-perovskite phase transition. <i>Earth, Planets and Space</i> , 2005 , 57, 459-464	2.9	21
The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO3. <i>Earth and Planetary Science Letters</i> , 2005 , 230, 1-10	5.3	129
Elasticity of (Mg, Fe)(Si, Al)O3-perovskite at high pressure. <i>Earth and Planetary Science Letters</i> , 2005 , 240, 529-536	5.3	38
Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	42
High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al2O3. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	35
Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. <i>Nature</i> , 2005 , 438, 1004-7	50.4	175
Simulation of hydrated Li+-, Na+- and K+-montmorillonite/polymer nanocomposites using large-scale molecular dynamics. <i>Chemical Physics Letters</i> , 2004 , 389, 261-267	2.5	42
Density-Functional-Theory-Based Study of the Dehydroxylation Behavior of Aluminous Dioctahedral 2:1 Layer-Type Clay Minerals. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 9685-9694	3.4	39
A Density Functional Theory Study of Catalytic trans-Esterification by tert-Butoxide MgAl Anionic Clays. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 3476-3485	3.4	59
Study of Thermally Treated Lithium Montmorillonite by Ab Initio Methods. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 12470-12477	3.4	29
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. <i>Perkin Transactions II RSC</i> , 2002 , 1238-1245		13
Plane-wave density functional theoretic study of formation of clay-polymer nanocomposite materials by self-catalyzed in situ intercalative polymerization. <i>Journal of the American Chemical Society</i> , 2001 , 123, 11764-74	16.4	75
A New Design Strategy for Molecular Recognition in Heterogeneous Systems: A Universal Crystal-Face Growth Inhibitor for Barium Sulfate. <i>Journal of the American Chemical Society</i> , 2000 , 122, 11557-11558	16.4	60
	Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO3 post-perovskite. <i>Geophysical Research Letters</i> , 2006, 33, Shear-induced material transfer across the core-mantle boundary aided by the post-perovskite phase transition. <i>Earth, Planets and Space</i> , 2005, 57, 459-464 The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO3. <i>Earth and Planetary Science Letters</i> , 2005, 230, 1-10 Elasticity of (Mg, Fe)(Si, Al)O3-perovskite at high pressure. <i>Earth and Planetary Science Letters</i> , 2005, 230, 1-10 Elasticity os in state of ferric iron in Al-bearing perovskite in the lower mantle. <i>Geophysical Research Letters</i> , 2005, 32, High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al2O3. <i>Geophysical Research Letters</i> , 2005, 32, Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. <i>Nature</i> , 2005, 438, 1004-7 Simulation of hydrated Li+-, Na+- and K+-montmorillonite/polymer nanocomposites using large-scale molecular dynamics. <i>Chemical Physics Letters</i> , 2004, 389, 261-267 Density-Functional-Theory-Based Study of the Dehydroxylation Behavior of Aluminous Dioctahedral 2:1 Layer-Type Clay Minerals. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9685-9694 A Density Functional Theory Study of Catalytic trans-Esterification by tert-Butoxide MgAl Anionic Clays. <i>Journal of Physical Chemistry B</i> , 2002, 106, 12470-12477 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. <i>Perkin Transactions IR SC</i> , 2002, 1238-1245 Plane-wave density functional theoretic study of formation of clay-polymer nanocomposite materials by self-catalyzed in situ intercalative polymerization. <i>Journal of the American Chemical Society</i> , 2000, 123, 11764-74 A New Design Strategy for Molecular Recognition in Heterogeneous Systems:Ila Universal Crystal-Face Growth	Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO3 post-perovskite. <i>Geophysical Research Letters</i> , 2006 , 33, 49 Shear-induced material transfer across the core-mantle boundary aided by the post-perovskite phase transition. <i>Earth, Planets and Space</i> , 2005 , 57, 459-464 The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO3. <i>Earth and Planetary Science Letters</i> , 2005 , 230, 1-10 53 Elasticity of (Mg, Fe)(Si, Al)O3-perovskite at high pressure. <i>Earth and Planetary Science Letters</i> , 2005 , 240, 529-536 Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. <i>Geophysical Research Letters</i> , 2005 , 32, High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al2O3. <i>Geophysical Research Letters</i> , 2005 , 32, Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties. <i>Nature</i> , 2005 , 438, 1004-7 Simulation of hydrated Li+-, Na+- and K+-montmorillonite/polymer nanocomposites using large-scale molecular dynamics. <i>Chemical Physics Letters</i> , 2004 , 389, 261-267 Density-Functional-Theory-Based Study of the Dehydroxylation Behavior of Aluminous Dioctahedral 2:1 Layer-Type Clay Minerals. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 9685-9694 A Density Functional Theory Study of Catalytic trans-Esterification by tert-Butoxide MgAl Anionic Clays. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 3476-3485 Study of Thermally Treated Lithium Montmorillonite by Ab Initio Methods. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 12470-12477 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. <i>Perkin Transactions IRSC</i> , 2002 , 1238-1245 Plane-wave density functional theoretic study of formation of clay-polymer nanocomposite materials by self-catalyzed in situ intercalative polymerization. <i>Journal </i>