David M Sherman

List of Publications by Year
in descending order

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76	5,848	66234	74018
papers	citations	42 h-index	75 g-index

80	80	80	5625
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Natural attenuation of lead by microbial manganese oxides in a karst aquifer. Science of the Total Environment, 2021, 754, 142312.	3.9	11
2	Molecular speciation of Mo (VI) on goethite and its implications for molybdenum and its isotopic cycle in ocean. Geochimica Et Cosmochimica Acta, 2021, 313, 116-132.	1.6	6
3	Isotopic disequilibrium of Cu in marine ferromanganese crusts: Evidence from ab initio predictions of Cu isotope fractionation on sorption to birnessite. Earth and Planetary Science Letters, 2020, 549, 116540.	1.8	17
4	The nature of NaClâ€“H2O deep fluids from ab initio molecular dynamics at 0.5â€“4.5â€¯GPa, 20â€“800â€¯Â°C, and 1â€“14â€¯m NaCl. Geochimica Et Cosmochimica Acta, 2020, 277, 243-264.	1.6	3
5	The solubility of goethite with structurally incorporated nickel and cobalt: Implication for laterites. Chemical Geology, 2019, 518, 1-8.	1.4	9
6	Sorption of nickel ontogoethite (Î±-FeOOH) and desorption kinetics of aged synthetic Ni-goethite: Implication for Ni laterite ore. Chemical Geology, 2019, 509, 223-233.	1.4	15
7	Spectral reflectance properties of magnetites: Implications for remote sensing. Icarus, 2019, 319, 525-539.	1.1	40
8	The dissociation mechanism and thermodynamic properties of HCl(aq) in hydrothermal fluids (to) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 226, 84-106.	1.6	29
9	Fate of As(III) and As(V) during Microbial Reduction of Arsenic-Bearing Ferrihydrite Facilitated by Activated Carbon. ACS Earth and Space Chemistry, 2018, 2, 878-887.	1.2	30
10	Irreversibility of sorption of cobalt to goethite (Î±-FeOOH) and disparities in dissolution of aged synthetic Co-goethite. Chemical Geology, 2017, 467, 168-176.	1.4	16
11	A review of the coordination chemistry of hydrothermal systems, or do coordination changes make ore deposits?. Chemical Geology, 2016, 447, 219-253.	1.4	177
12	Speciation and thermodynamic properties of zinc in sulfur-rich hydrothermal fluids: Insights from ab initio molecular dynamics simulations and X-ray absorption spectroscopy. Geochimica Et Cosmochimica Acta, 2016, 179, 32-52.	1.6	27
13	Reply to comment on â€œMolecular controls on Cu and Zn isotopic fractionation in Feâ€“Mn crustsâ€• Earth and Planetary Science Letters, 2015, 411, 313-315.	1.8	8
14	Zinc complexation in chloride-rich hydrothermal fluids (25â€“600 Â°C): A thermodynamic model derived from ab initio molecular dynamics. Geochimica Et Cosmochimica Acta, 2015, 150, 265-284.	1.6	85
15	Palladium complexation in chloride- and bisulfide-rich fluids: Insights from ab initio molecular dynamics simulations and X-ray absorption spectroscopy. Geochimica Et Cosmochimica Acta, 2015, 161, 128-145.	1.6	55
16	Metal complexation and ion hydration in low density hydrothermal fluids: Ab initio molecular dynamics simulation of Cu(I) and Au(I) in chloride solutions (25â€“1000Â°C, 1â€“5000bar). Geochimica Et Cosmochimica Acta, 2014, 131, 196-212.	1.6	69
17	Complexation of gold in S3â^'-rich hydrothermal fluids: Evidence from ab-initio molecular dynamics simulations. Chemical Geology, 2013, 347, 34-42.	1.4	40
18	Ab initio molecular dynamics simulation and free energy exploration of copper(I) complexation by chloride and bisulfide in hydrothermal fluids. Geochimica Et Cosmochimica Acta, 2013, 102, 45-64.	1.6	79

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19	Equilibrium isotopic fractionation of copper during oxidation/reduction, aqueous complexation and ore-forming processes: Predictions from hybrid density functional theory. Geochimica Et Cosmochimica Acta, 2013, 118, 85-97.	1.6	79
20	Speciation of nickel (II) chloride complexes in hydrothermal fluids: In situ XAS study. Chemical Geology, 2012, 334, 345-363.	1.4	69
21	Metal complexation and ion association in hydrothermal fluids: insights from quantum chemistry and molecular dynamics. Geofluids, 2010, 10, 41-57.	0.3	16
22	Surface complexation of Cu on birnessite (Î´-MnO2): Controls on Cu in the deep ocean. Geochimica Et Cosmochimica Acta, 2010, 74, 6721-6730.	1.6	91
23	5. Surface Complexation Modeling: Mineral Fluid Equilbria at the Molecular Scale. , 2009, , 181-206.		3
24	Electronic structures of siderite (FeCO3) and rhodochrosite (MnCO3): Oxygen K-edge spectroscopy and hybrid density functional theory. American Mineralogist, 2009, 94, 166-171.	0.9	21
25	Surface Complexation Modeling: Mineral Fluid Equilbria at the Molecular Scale. Reviews in Mineralogy and Geochemistry, 2009, 70, 181-205.	2.2	14
26	Surface complexation of U(VI) on goethite (Î±-FeOOH). Geochimica Et Cosmochimica Acta, 2008, 72, 298-310.	1.6	186
27	Sorption of As(III) and As(V) to siderite, green rust (fougerite) and magnetite: Implications for arsenic release in anoxic groundwaters. Chemical Geology, 2008, 255, 173-181.	1.4	212
28	Sorption of Ni by birnessite: Equilibrium controls on Ni in seawater. Chemical Geology, 2007, 238, 94-106.	1.4	165
29	Complexation of Cu+ in Hydrothermal NaCl Brines: Ab initio molecular dynamics and energetics. Geochimica Et Cosmochimica Acta, 2007, 71, 714-722.	1.6	67
30	Crystal-chemistry of Ni in marine ferromanganese crusts and nodules. American Mineralogist, 2007, 92, 1087-1092.	0.9	91
31	Surface complexation model for multisite adsorption of copper(II) onto kaolinite. Geochimica Et Cosmochimica Acta, 2005, 69, 3733-3745.	1.6	81
32	Electronic structures of iron(III) and manganese(IV) (hydr)oxide minerals: Thermodynamics of photochemical reductive dissolution in aquatic environments. Geochimica Et Cosmochimica Acta, 2005, 69, 3249-3255.	1.6	212
33	Vanadium(V) adsorption onto goethite (Î±-FeOOH) at pH 1.5 to 12: a surface complexation model based on ab initio molecular geometries and EXAFS spectroscopy. Geochimica Et Cosmochimica Acta, 2004, 68, 1723-1733.	1.6	240
34	Copper(II) sorption onto goethite, hematite and lepidocrocite: a surface complexation model based on ab initio molecular geometries and EXAFS spectroscopy. Geochimica Et Cosmochimica Acta, 2004, 68, 2623-2637.	1.6	194
35	Zinc Complexation in Hydrothermal Chloride Brines:Â Results from ab Initio Molecular Dynamics Calculations. Journal of Physical Chemistry A, 2003, 107, 1050-1054.	1.1	29
36	Hydration of Sr2 +in Hydrothermal Solutions from ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2003, 107, 9056-9058.	1.2	37

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37	Surface oxidation of pyrite under ambient atmospheric and aqueous (pH = 2 to 10) conditions: electronic structure and mineralogy from X-ray absorption spectroscopy. Geochimica Et Cosmochimica Acta, 2003, 67, 881-893.	1.6	152
38	Surface oxidation of chalcopyrite (CuFeS2) under ambient atmospheric and aqueous (pH 2-10) conditions: Cu, Fe L- and O K-edge X-ray spectroscopy. Geochimica Et Cosmochimica Acta, 2003, 67, 2137-2146.	1.6	125
39	Surface complexation of arsenic(V) to iron(III) (hydr)oxides: structural mechanism from ab initio molecular geometries and EXAFS spectroscopy. Geochimica Et Cosmochimica Acta, 2003, 67, 4223-4230.	1.6	624
40	Surface oxidation of chalcocite (Cu₂S) under aqueous (pH = 2â€“11) and ambient atmospheric conditions: Mineralogy from CuL- and OK-edge X-ray absorption spectroscopy. American Mineralogist, 2003, 88, 1652-1656.	0.9	30
41	The reduction of aqueous Au³⁺by sulfide minerals and green rust phases. American Mineralogist, 2003, 88, 725-739.	0.9	21
42	Incorporation of Cr, Mn and Ni into goethite (Î±-FeOOH): mechanism from extended X-ray absorption fine structure spectroscopy. Clay Minerals, 2002, 37, 639-649.	0.2	90
43	Ion association in concentrated NaCl brines from ambient to supercritical conditions: results from classical molecular dynamics simulations. Geochemical Transactions, 2002, 3, 1.	1.8	75
44	Quantum Chemistry and Classical Simulations of Metal Complexes in Aqueous Solutions. Reviews in Mineralogy and Geochemistry, 2001, 42, 273-317.	2.2	15
45	Sorption of As(V) on green rust (Fe4(II)Fe2(III)(OH)12SO4 Â· 3H2O) and lepidocrocite (Î³-FeOOH): Surface complexes from EXAFS spectroscopy. Geochimica Et Cosmochimica Acta, 2001, 65, 1015-1023.	1.6	166
46	8. Quantum Chemistry and Classical Simulations of Metal Complexes in Aqueous Solutions. , 2001, , 273-318.		4
47	Molecular Dynamics simulation of aqueous ZnC12solutions. Molecular Physics, 2001, 99, 825-833.	0.8	37
48	Structural Chemistry of Fe, Mn, and Ni in Synthetic Hematites as Determined by Extended X-Ray Absorption Fine Structure Spectroscopy. Clays and Clay Minerals, 2000, 48, 521-527.	0.6	55
49	Complexation of Cu2+ in oxidized NaCl brines from 25Â°C to 175Â°C: results from in situ EXAFS spectroscopy. Chemical Geology, 2000, 167, 65-73.	1.4	55
50	Antimony transport in hydrothermal solutions: an EXAFS study of antimony(V) complexation in alkaline sulfide and sulfideâ€“chloride brines at temperatures from 25Â°C to 300Â°C at Psat. Chemical Geology, 2000, 167, 161-167.	1.4	42
51	Speciation of tin (Sn2+ and Sn4+) in aqueous Cl solutions from 25Â°C to 350Â°C: an in situ EXAFS study. Chemical Geology, 2000, 167, 169-176.	1.4	56
52	Surface Complexation of Hg2+ on Goethite: Mechanism from EXAFS Spectroscopy and Density Functional Calculations. Journal of Colloid and Interface Science, 1999, 219, 345-350.	5.0	61
53	Effect of inorganic and organic ligands on the mechanism of cadmium sorption to goethite. Geochimica Et Cosmochimica Acta, 1999, 63, 2989-3002.	1.6	193
54	The mechanism of cadmium surface complexation on iron oxyhydroxide minerals. Geochimica Et Cosmochimica Acta, 1999, 63, 2971-2987.	1.6	175

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55	An EXAFS spectroscopic study of aqueous antimony(III)-chloride complexation at temperatures from 25 to 250Â°C. Chemical Geology, 1998, 151, 21-27.	1.4	37
56	Aqueous speciation of yttrium at temperatures from 25 to 340Â°C at Psat: an in situ EXAFS study. Chemical Geology, 1998, 151, 29-39.	1.4	47
57	An extended X-ray absorption fine structure spectroscopy investigation of cadmium sorption on cryptomelane (KMn8O16). Chemical Geology, 1998, 151, 95-106.	1.4	59
58	The Adsorption Mechanism of Sr²⁺ on the Surface of Goethite. Radiochimica Acta, 1998, 81, 201-206.	0.5	32
59	The composition of the Earth's core: constraints on S and Si vs. temperature. Earth and Planetary Science Letters, 1997, 153, 149-155.	1.8	42
60	Reinvestigation of the annite = sanidine+magnetite+H2reaction using the fH2-sensor technique. American Mineralogist, 1996, 81, 475-484.	0.9	9
61	Mineralogical and geochemical evolution of micas from miarolitic pegmatites of the anorogenic pikes peak batholith, Colorado. Mineralogy and Petrology, 1995, 55, 1-26.	0.4	57
62	Stability of possible Fe-FeS and Fe-FeO alloy phases at high pressure and the composition of the Earth's core. Earth and Planetary Science Letters, 1995, 132, 87-98.	1.8	71
63	First-principles prediction of the high-pressure phase transition and electronic structure of FeO: Implications for the chemistry of the lower mantle and core. Geophysical Research Letters, 1995, 22, 1001-1004.	1.5	42
64	Equation of state and highâ€pressure phase transitions of stishovite (SiO₂): Ab initio (periodic Hartreeâ€Fock) results. Journal of Geophysical Research, 1993, 98, 11865-11873.	3.3	20
65	Equation of state, elastic properties, and stability of CaSiO₃ perovskite: First principles (periodic Hartreeâ€Fock) results. Journal of Geophysical Research, 1993, 98, 19795-19805.	3.3	25
66	Evidence for Ammonium-Bearing Minerals on Ceres. Science, 1992, 255, 1551-1553.	6.0	151
67	The highâ€pressure electronic structure of magnesiowustite (Mg, Fe)O: Applications to the physics and chemistry of the lower mantle. Journal of Geophysical Research, 1991, 96, 14299-14312.	3.3	52
68	Chemical bonding in the outer core: Highâ€pressure electronic structures of oxygen and sulfur in metallic iron. Journal of Geophysical Research, 1991, 96, 18029-18036.	3.3	12
69	Chemical bonding and the incorporation of potassium into the Earth's core. Geophysical Research Letters, 1990, 17, 693-696.	1.5	18
70	The nature of the pressureâ€induced metallization of FeO and its implications to the coreâ€mantle boundary. Geophysical Research Letters, 1989, 16, 515-518.	1.5	20
71	Molecular orbital (SCF-X?-SW) theory of metal-metal charge transfer processes in minerals. Physics and Chemistry of Minerals, 1987, 14, 355-363.	0.3	92
72	Molecular orbital (SCF-X?-SW) theory of metal-metal charge transfer processes in minerals. Physics and Chemistry of Minerals, 1987, 14, 364-367.	0.3	45

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73	Cluster molecular orbital description of the electronic structures of mixed-valence iron oxides and silicates. Solid State Communications, 1986, 58, 719-723.	0.9	15
74	The electronic structures of Fe3+ coordination sites in iron oxides: Applications to spectra, bonding, and magnetism. Physics and Chemistry of Minerals, 1985, 12, 161-175.	0.3	214
75	SCF-X?-SW MO Study of Fe-O and Fe-OH chemical bonds; applications to the mï¿½ssbauer spectra and magnetochemistry of hydroxyl-bearing Fe3+ oxides and silicates. Physics and Chemistry of Minerals, 1985, 12, 311-314.	0.3	19
76	Spectral characteristics of the iron oxides with application to the Martian bright region mineralogy. Journal of Geophysical Research, 1982, 87, 10169-10180.	3.3	128