

David M Sherman

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8060005/publications.pdf>

Version: 2024-02-01

76
papers

5,848
citations

66234

42
h-index

74018

75
g-index

80
all docs

80
docs citations

80
times ranked

5625
citing authors

#	ARTICLE	IF	CITATIONS
1	Surface complexation of arsenic(V) to iron(III) (hydr)oxides: structural mechanism from ab initio molecular geometries and EXAFS spectroscopy. <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 4223-4230.	1.6	624
2	Vanadium(V) adsorption onto goethite (\hat{I}^{\pm} -FeOOH) at pH 1.5 to 12: a surface complexation model based on ab initio molecular geometries and EXAFS spectroscopy. <i>Geochimica Et Cosmochimica Acta</i> , 2004, 68, 1723-1733.	1.6	240
3	The electronic structures of Fe ³⁺ coordination sites in iron oxides: Applications to spectra, bonding, and magnetism. <i>Physics and Chemistry of Minerals</i> , 1985, 12, 161-175.	0.3	214
4	Electronic structures of iron(III) and manganese(IV) (hydr)oxide minerals: Thermodynamics of photochemical reductive dissolution in aquatic environments. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 3249-3255.	1.6	212
5	Sorption of As(III) and As(V) to siderite, green rust (fougerite) and magnetite: Implications for arsenic release in anoxic groundwaters. <i>Chemical Geology</i> , 2008, 255, 173-181.	1.4	212
6	Copper(II) sorption onto goethite, hematite and lepidocrocite: a surface complexation model based on ab initio molecular geometries and EXAFS spectroscopy. <i>Geochimica Et Cosmochimica Acta</i> , 2004, 68, 2623-2637.	1.6	194
7	Effect of inorganic and organic ligands on the mechanism of cadmium sorption to goethite. <i>Geochimica Et Cosmochimica Acta</i> , 1999, 63, 2989-3002.	1.6	193
8	Surface complexation of U(VI) on goethite (\hat{I}^{\pm} -FeOOH). <i>Geochimica Et Cosmochimica Acta</i> , 2008, 72, 298-310.	1.6	186
9	A review of the coordination chemistry of hydrothermal systems, or do coordination changes make ore deposits?. <i>Chemical Geology</i> , 2016, 447, 219-253.	1.4	177
10	The mechanism of cadmium surface complexation on iron oxyhydroxide minerals. <i>Geochimica Et Cosmochimica Acta</i> , 1999, 63, 2971-2987.	1.6	175
11	Sorption of As(V) on green rust (Fe ₄ (II)Fe ₂ (III)(OH) ₁₂ SO ₄ · 3H ₂ O) and lepidocrocite (\hat{I}^{\pm} -FeOOH): Surface complexes from EXAFS spectroscopy. <i>Geochimica Et Cosmochimica Acta</i> , 2001, 65, 1015-1023.	1.6	166
12	Sorption of Ni by birnessite: Equilibrium controls on Ni in seawater. <i>Chemical Geology</i> , 2007, 238, 94-106.	1.4	165
13	Surface oxidation of pyrite under ambient atmospheric and aqueous (pH = 2 to 10) conditions: electronic structure and mineralogy from X-ray absorption spectroscopy. <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 881-893.	1.6	152
14	Evidence for Ammonium-Bearing Minerals on Ceres. <i>Science</i> , 1992, 255, 1551-1553.	6.0	151
15	Spectral characteristics of the iron oxides with application to the Martian bright region mineralogy. <i>Journal of Geophysical Research</i> , 1982, 87, 10169-10180.	3.3	128
16	Surface oxidation of chalcopyrite (CuFeS ₂) under ambient atmospheric and aqueous (pH 2-10) conditions: Cu, Fe L- and O K-edge X-ray spectroscopy. <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 2137-2146.	1.6	125
17	Molecular orbital (SCF-X?SW) theory of metal-metal charge transfer processes in minerals. <i>Physics and Chemistry of Minerals</i> , 1987, 14, 355-363.	0.3	92
18	Crystal-chemistry of Ni in marine ferromanganese crusts and nodules. <i>American Mineralogist</i> , 2007, 92, 1087-1092.	0.9	91

#	ARTICLE	IF	CITATIONS
19	Surface complexation of Cu on birnessite ($\hat{\Gamma}$ -MnO ₂): Controls on Cu in the deep ocean. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 6721-6730.	1.6	91
20	Incorporation of Cr, Mn and Ni into goethite ($\hat{\Gamma}$ -FeOOH): mechanism from extended X-ray absorption fine structure spectroscopy. <i>Clay Minerals</i> , 2002, 37, 639-649.	0.2	90
21	Zinc complexation in chloride-rich hydrothermal fluids (25–600 °C): A thermodynamic model derived from ab initio molecular dynamics. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 150, 265-284.	1.6	85
22	Surface complexation model for multisite adsorption of copper(II) onto kaolinite. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 3733-3745.	1.6	81
23	Ab initio molecular dynamics simulation and free energy exploration of copper(I) complexation by chloride and bisulfide in hydrothermal fluids. <i>Geochimica Et Cosmochimica Acta</i> , 2013, 102, 45-64.	1.6	79
24	Equilibrium isotopic fractionation of copper during oxidation/reduction, aqueous complexation and ore-forming processes: Predictions from hybrid density functional theory. <i>Geochimica Et Cosmochimica Acta</i> , 2013, 118, 85-97.	1.6	79
25	Ion association in concentrated NaCl brines from ambient to supercritical conditions: results from classical molecular dynamics simulations. <i>Geochemical Transactions</i> , 2002, 3, 1.	1.8	75
26	Stability of possible Fe-FeS and Fe-FeO alloy phases at high pressure and the composition of the Earth's core. <i>Earth and Planetary Science Letters</i> , 1995, 132, 87-98.	1.8	71
27	Speciation of nickel (II) chloride complexes in hydrothermal fluids: In situ XAS study. <i>Chemical Geology</i> , 2012, 334, 345-363.	1.4	69
28	Metal complexation and ion hydration in low density hydrothermal fluids: Ab initio molecular dynamics simulation of Cu(I) and Au(I) in chloride solutions (25–1000 °C, 1–5000 bar). <i>Geochimica Et Cosmochimica Acta</i> , 2014, 131, 196-212.	1.6	69
29	Complexation of Cu ⁺ in Hydrothermal NaCl Brines: Ab initio molecular dynamics and energetics. <i>Geochimica Et Cosmochimica Acta</i> , 2007, 71, 714-722.	1.6	67
30	Surface Complexation of Hg ²⁺ on Goethite: Mechanism from EXAFS Spectroscopy and Density Functional Calculations. <i>Journal of Colloid and Interface Science</i> , 1999, 219, 345-350.	5.0	61
31	An extended X-ray absorption fine structure spectroscopy investigation of cadmium sorption on cryptomelane (KMn ₈ O ₁₆). <i>Chemical Geology</i> , 1998, 151, 95-106.	1.4	59
32	Mineralogical and geochemical evolution of micas from miarolitic pegmatites of the anorogenic pikes peak batholith, Colorado. <i>Mineralogy and Petrology</i> , 1995, 55, 1-26.	0.4	57
33	Speciation of tin (Sn ²⁺ and Sn ⁴⁺) in aqueous Cl solutions from 25 °C to 350 °C: an in situ EXAFS study. <i>Chemical Geology</i> , 2000, 167, 169-176.	1.4	56
34	Structural Chemistry of Fe, Mn, and Ni in Synthetic Hematites as Determined by Extended X-Ray Absorption Fine Structure Spectroscopy. <i>Clays and Clay Minerals</i> , 2000, 48, 521-527.	0.6	55
35	Complexation of Cu ²⁺ in oxidized NaCl brines from 25 °C to 175 °C: results from in situ EXAFS spectroscopy. <i>Chemical Geology</i> , 2000, 167, 65-73.	1.4	55
36	Palladium complexation in chloride- and bisulfide-rich fluids: Insights from ab initio molecular dynamics simulations and X-ray absorption spectroscopy. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 161, 128-145.	1.6	55

#	ARTICLE	IF	CITATIONS
37	The high-pressure electronic structure of magnesiowustite (Mg, Fe)O: Applications to the physics and chemistry of the lower mantle. <i>Journal of Geophysical Research</i> , 1991, 96, 14299-14312.	3.3	52
38	Aqueous speciation of yttrium at temperatures from 25 to 340°C at Psat: an in situ EXAFS study. <i>Chemical Geology</i> , 1998, 151, 29-39.	1.4	47
39	Molecular orbital (SCF-X?SW) theory of metal-metal charge transfer processes in minerals. <i>Physics and Chemistry of Minerals</i> , 1987, 14, 364-367.	0.3	45
40	First-principles prediction of the high-pressure phase transition and electronic structure of FeO: Implications for the chemistry of the lower mantle and core. <i>Geophysical Research Letters</i> , 1995, 22, 1001-1004.	1.5	42
41	The composition of the Earth's core: constraints on S and Si vs. temperature. <i>Earth and Planetary Science Letters</i> , 1997, 153, 149-155.	1.8	42
42	Antimony transport in hydrothermal solutions: an EXAFS study of antimony(V) complexation in alkaline sulfide and sulfide-chloride brines at temperatures from 25°C to 300°C at Psat. <i>Chemical Geology</i> , 2000, 167, 161-167.	1.4	42
43	Complexation of gold in S ³⁺ -rich hydrothermal fluids: Evidence from ab-initio molecular dynamics simulations. <i>Chemical Geology</i> , 2013, 347, 34-42.	1.4	40
44	Spectral reflectance properties of magnetites: Implications for remote sensing. <i>Icarus</i> , 2019, 319, 525-539.	1.1	40
45	An EXAFS spectroscopic study of aqueous antimony(III)-chloride complexation at temperatures from 25 to 250°C. <i>Chemical Geology</i> , 1998, 151, 21-27.	1.4	37
46	Molecular Dynamics simulation of aqueous ZnCl ₂ solutions. <i>Molecular Physics</i> , 2001, 99, 825-833.	0.8	37
47	Hydration of Sr ²⁺ in Hydrothermal Solutions from ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2003, 107, 9056-9058.	1.2	37
48	The Adsorption Mechanism of Sr ²⁺ on the Surface of Goethite. <i>Radiochimica Acta</i> , 1998, 81, 201-206.	0.5	32
49	Surface oxidation of chalcocite (Cu ₂ S) under aqueous (pH = 2-11) and ambient atmospheric conditions: Mineralogy from Cu L _{2,3} - and O K ₁ -edge X-ray absorption spectroscopy. <i>American Mineralogist</i> , 2003, 88, 1652-1656.	0.9	30
50	Fate of As(III) and As(V) during Microbial Reduction of Arsenic-Bearing Ferrihydrite Facilitated by Activated Carbon. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 878-887.	1.2	30
51	Zinc Complexation in Hydrothermal Chloride Brines: Results from ab Initio Molecular Dynamics Calculations. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1050-1054.	1.1	29
52	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
53	Speciation and thermodynamic properties of zinc in sulfur-rich hydrothermal fluids: Insights from ab initio molecular dynamics simulations and X-ray absorption spectroscopy. <i>Geochimica Et Cosmochimica Acta</i> , 2016, 179, 32-52.	1.6	27
54	Equation of state, elastic properties, and stability of CaSiO ₃ perovskite: First principles (periodic Hartree-Fock) results. <i>Journal of Geophysical Research</i> , 1993, 98, 19795-19805.	3.3	25

#	ARTICLE	IF	CITATIONS
55	The reduction of aqueous Au ³⁺ by sulfide minerals and green rust phases. <i>American Mineralogist</i> , 2003, 88, 725-739.	0.9	21
56	Electronic structures of siderite (FeCO ₃) and rhodochrosite (MnCO ₃): Oxygen K-edge spectroscopy and hybrid density functional theory. <i>American Mineralogist</i> , 2009, 94, 166-171.	0.9	21
57	The nature of the pressure-induced metallization of FeO and its implications to the core-mantle boundary. <i>Geophysical Research Letters</i> , 1989, 16, 515-518.	1.5	20
58	Equation of state and high-pressure phase transitions of stishovite (SiO ₂): Ab initio (periodic Hartree-Fock) results. <i>Journal of Geophysical Research</i> , 1993, 98, 11865-11873.	3.3	20
59	SCF-X ² -SW MO Study of Fe-O and Fe-OH chemical bonds; applications to the Mössbauer spectra and magnetochemistry of hydroxyl-bearing Fe ³⁺ oxides and silicates. <i>Physics and Chemistry of Minerals</i> , 1985, 12, 311-314.	0.3	19
60	Chemical bonding and the incorporation of potassium into the Earth's core. <i>Geophysical Research Letters</i> , 1990, 17, 693-696.	1.5	18
61	Isotopic disequilibrium of Cu in marine ferromanganese crusts: Evidence from ab initio predictions of Cu isotope fractionation on sorption to birnessite. <i>Earth and Planetary Science Letters</i> , 2020, 549, 116540.	1.8	17
62	Metal complexation and ion association in hydrothermal fluids: insights from quantum chemistry and molecular dynamics. <i>Geofluids</i> , 2010, 10, 41-57.	0.3	16
63	Irreversibility of sorption of cobalt to goethite (±-FeOOH) and disparities in dissolution of aged synthetic Co-goethite. <i>Chemical Geology</i> , 2017, 467, 168-176.	1.4	16
64	Cluster molecular orbital description of the electronic structures of mixed-valence iron oxides and silicates. <i>Solid State Communications</i> , 1986, 58, 719-723.	0.9	15
65	Quantum Chemistry and Classical Simulations of Metal Complexes in Aqueous Solutions. <i>Reviews in Mineralogy and Geochemistry</i> , 2001, 42, 273-317.	2.2	15
66	Sorption of nickel onto goethite (±-FeOOH) and desorption kinetics of aged synthetic Ni-goethite: Implication for Ni laterite ore. <i>Chemical Geology</i> , 2019, 509, 223-233.	1.4	15
67	Surface Complexation Modeling: Mineral Fluid Equilibria at the Molecular Scale. <i>Reviews in Mineralogy and Geochemistry</i> , 2009, 70, 181-205.	2.2	14
68	Chemical bonding in the outer core: High-pressure electronic structures of oxygen and sulfur in metallic iron. <i>Journal of Geophysical Research</i> , 1991, 96, 18029-18036.	3.3	12
69	Natural attenuation of lead by microbial manganese oxides in a karst aquifer. <i>Science of the Total Environment</i> , 2021, 754, 142312.	3.9	11
70	Reinvestigation of the annite = sanidine+magnetite+H ₂ reaction using the fH ₂ -sensor technique. <i>American Mineralogist</i> , 1996, 81, 475-484.	0.9	9
71	The solubility of goethite with structurally incorporated nickel and cobalt: Implication for laterites. <i>Chemical Geology</i> , 2019, 518, 1-8.	1.4	9
72	Reply to comment on "Molecular controls on Cu and Zn isotopic fractionation in Fe-Mn crusts". <i>Earth and Planetary Science Letters</i> , 2015, 411, 313-315.	1.8	8

#	ARTICLE	IF	CITATIONS
73	Molecular speciation of Mo (VI) on goethite and its implications for molybdenum and its isotopic cycle in ocean. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 313, 116-132.	1.6	6
74	8. Quantum Chemistry and Classical Simulations of Metal Complexes in Aqueous Solutions. , 2001, , 273-318.		4
75	5. Surface Complexation Modeling: Mineral Fluid Equilibria at the Molecular Scale. , 2009, , 181-206.		3
76	The nature of NaCl-H ₂ O deep fluids from ab initio molecular dynamics at 0.5-4.5 GPa, 20-800°C, and 1-14 m NaCl. <i>Geochimica Et Cosmochimica Acta</i> , 2020, 277, 243-264.	1.6	3