Kevin M Rosso

List of Publications by Year in Descending Order

335 papers	13,508 citations	57 h-index	100 g-index
356 ext. papers	15,513 ext. citations	6.1 avg, IF	6.65 L-index

#	Paper	IF	Citations
335	Understanding Competitive Phosphate and Silicate Adsorption on Goethite by Connecting Batch Experiments with Density Functional Theory Calculations.. *Environmental Science & Technology*, **2022**, 56, 823-834	10.3	2
334	Electron-Stimulated Formation and Release of Molecular Hydrogen and Oxygen from Boehmite Nanoplatelet Films. *Journal of Physical Chemistry C*, **2022**, 126, 2542-2547	3.8	
333	Understanding the Importance of Labile Fe(III) during Fe(II)-Catalyzed Transformation of Metastable Iron Oxyhydroxides.. *Environmental Science & Technology*, **2022**,	10.3	3
332	Ab Initio Evaluation of Solid-State Transformation Pathways from Ferrihydrite to Goethite. *ACS Earth and Space Chemistry*, **2022**, 6, 800-809	3.2	
331	Particle-based hematite crystallization is invariant to initial particle morphology.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2112679119	11.5	2
330	No Hydrogen Bonding between Water and Hydrophilic Single Crystal MgO Surfaces?. *Journal of Physical Chemistry C*, **2021**, 125, 26132-26138	3.8	2
329	Theory-Guided Inelastic Neutron Scattering of Crystalline Alkaline Aluminate Salts Bearing Principal Motifs of Solution-State Species. *Inorganic Chemistry*, **2021**, 60, 16223-16232	5.1	1
328	Molecular Examination of Ion-Pair Competition in Alkaline Aluminate Solutions Using In Situ Liquid SIMS. *Analytical Chemistry*, **2021**, 93, 1068-1075	7.8	1
327	Predicting the temperature dependence of self-diffusion behavior in Ni-Cr alloys via molecular dynamics. *Materials Today Communications*, **2021**, 26, 101982	2.5	1
326	Combined multiplet theory and experiment for the Fe 2p and 3p XPS of FeO and FeO. *Journal of Chemical Physics*, **2021**, 154, 094709	3.9	14
325	The Steady March toward Biomimetic Nanoelectronics. *ACS Nano*, **2021**, 15, 7844-7847	16.7	0
324	Reversible ketone hydrogenation and dehydrogenation for aqueous organic redox flow batteries. *Science*, **2021**, 372, 836-840	33.3	40
323	Crystallization and Phase Transformations of Aluminum (Oxy)hydroxide Polymorphs in Caustic Aqueous Solution. *Inorganic Chemistry*, **2021**, 60, 9820-9832	5.1	6
322	Fe(II) Redox Chemistry in the Environment. *Chemical Reviews*, **2021**, 121, 8161-8233	68.1	37
321	Hydroxide promotes ion pairing in the NaNO-NaOH-HO system. *Physical Chemistry Chemical Physics*, **2021**, 23, 112-122	3.6	3
320	Facet-Dependent Photodegradation of Methylene Blue by Hematite Nanoplates in Visible Light. *Environmental Science & Technology*, **2021**, 55, 677-688	10.3	26
319	Self-similar mesocrystals form via interface-driven nucleation and assembly. *Nature*, **2021**, 590, 416-422	50.4	33

318	Ab initio thermodynamics reveals the nanocomposite structure of ferrihydrite. *Communications Chemistry*, **2021**, 4,	6.3	4
317	Labile Fe(III) supersaturation controls nucleation and properties of product phases from Fe(II)-catalyzed ferrihydrite transformation. *Geochimica Et Cosmochimica Acta*, **2021**, 309, 272-285	5.5	2
316	Cluster defects in gibbsite nanoplates grown at acidic to neutral pH. *Nanoscale*, **2021**, 13, 17373-17385	7.7	0
315	The controlling role of atmosphere in dawsonite gibbsite precipitation from tetrahedral aluminate species. *Dalton Transactions*, **2021**, 50, 13438-13446	4.3	1
314	Citrate Controls Fe(II)-Catalyzed Transformation of Ferrihydrite by Complexation of the Labile Fe(III) Intermediate. *Environmental Science & Technology*, **2020**, 54, 7309-7319	10.3	20
313	Solid-State Recrystallization Pathways of Sodium Aluminate Hydroxy Hydrates. *Inorganic Chemistry*, **2020**, 59, 6857-6865	5.1	7
312	Vacancy ordering during selective oxidation of ╫NiAl. *Materialia*, **2020**, 12, 100783	3.2	4
311	Two-step route to size and shape controlled gibbsite nanoplates and the crystal growth mechanism. *CrystEngComm*, **2020**, 22, 2555-2565	3.3	6
310	Electronic and Vibrational Contributions to the Bulk Stabilities of Trivalent 3d Transition Metal Oxyhydroxides from Electronic Structure Calculations. *Journal of Physical Chemistry C*, **2020**, 124, 7500-7510	3.8	
309	Emerging investigator series: ion diffusivities in nanoconfined interfacial water films contribute to mineral carbonation thresholds. *Environmental Science: Nano*, **2020**, 7, 1068-1081	7.1	8
308	Photo-production of reactive oxygen species and degradation of dissolved organic matter by hematite nanoplates functionalized by adsorbed oxalate. *Environmental Science: Nano*, **2020**, 7, 2278-2292	7.1	12
307	Polaronic structure of excess electrons and holes for a series of bulk iron oxides. *Physical Chemistry Chemical Physics*, **2020**, 22, 10699-10709	3.6	6
306	Surface Hydration and Hydroxyl Configurations of Gibbsite and Boehmite Nanoplates. *Journal of Physical Chemistry C*, **2020**, 124, 5275-5285	3.8	13
305	Phase Transition and Liquid-like Superionic Conduction in Ag2S. *Journal of Physical Chemistry C*, **2020**, 124, 10150-10158	3.8	2
304	Connecting particle interactions to agglomerate morphology and rheology of boehmite nanocrystal suspensions. *Journal of Colloid and Interface Science*, **2020**, 572, 328-339	9.3	12
303	Correlating inter-particle forces and particle shape to shear-induced aggregation/fragmentation and rheology for dilute anisotropic particle suspensions: A complementary study via capillary rheometry and in-situ small and ultra-small angle X-ray scattering. *Journal of Colloid and Interface Science*, **2020**, 576, 47-58	9.3	10
302	Evolution of Radicals from the Photolysis of High Ionic Strength Alkaline Nitrite Solutions. *Journal of Physical Chemistry A*, **2020**, 124, 3019-3025	2.8	3
301	A Filon-like integration strategy for calculating exact exchange in periodic boundary conditions: a plane-wave DFT implementation. *Materials Theory*, **2020**, 4,	2.2	3

300	Electron transfer calculations between edge sharing octahedra in hematite, goethite, and annite. *Geochimica Et Cosmochimica Acta*, **2020**, 291, 79-91	5.5	6
299	The role of surface hydroxyls on the radiolysis of gibbsite and boehmite nanoplatelets. *Journal of Hazardous Materials*, **2020**, 398, 122853	12.8	8
298	Analysis of the Fe 2p XPS for hematite FeO: Consequences of covalent bonding and orbital splittings on multiplet splittings. *Journal of Chemical Physics*, **2020**, 152, 014704	3.9	27
297	Ion-ion interactions enhance aluminum solubility in alkaline suspensions of nano-gibbsite (Al(OH)) with sodium nitrite/nitrate. *Physical Chemistry Chemical Physics*, **2020**, 22, 4368-4378	3.6	7
296	Labile Fe(III) from sorbed Fe(II) oxidation is the key intermediate in Fe(II)-catalyzed ferrihydrite transformation. *Geochimica Et Cosmochimica Acta*, **2020**, 272, 105-120	5.5	26
295	Covalency in FeO and FeO: Consequences for XPS satellite intensity. *Journal of Chemical Physics*, **2020**, 153, 194702	3.9	9
294	Mechanisms of Al Dimerization in Alkaline Solutions. *Inorganic Chemistry*, **2020**, 59, 18181-18189	5.1	1
293	Influence of soluble oligomeric aluminum on precipitation in the Al-KOH-HO system. *Physical Chemistry Chemical Physics*, **2020**, 22, 24677-24685	3.6	4
292	Rethinking the magnetic properties of lepidocrocite: A density functional theory and cluster expansion study. *Journal of Applied Physics*, **2020**, 128, 103906	2.5	
291	Radiation-Induced Interfacial Hydroxyl Transformation on Boehmite and Gibbsite Basal Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 22185-22191	3.8	3
290	Nanoscale observations of Fe(II)-induced ferrihydrite transformation. *Environmental Science: Nano*, **2020**, 7, 2953-2967	7.1	8
289	Effect of Cr(III) Adsorption on the Dissolution of Boehmite Nanoparticles in Caustic Solution. *Environmental Science & Technology*, **2020**, 54, 6375-6384	10.3	2
288	Intermediate Species in the Crystallization of Sodium Aluminate Hydroxy Hydrates. *Journal of Physical Chemistry C*, **2020**, 124, 12337-12345	3.8	5
287	Inference of principal species in caustic aluminate solutions through solid-state spectroscopic characterization. *Dalton Transactions*, **2020**, 49, 5869-5880	4.3	6
286	Temperature Dependence of Self-Diffusion in Cr2O3 from First Principles. *Journal of Physical Chemistry C*, **2019**, 123, 22139-22150	3.8	6
285	Transformation of Gibbsite to Boehmite in Caustic Aqueous Solution at Hydrothermal Conditions. *Crystal Growth and Design*, **2019**, 19, 5557-5567	3.5	12
284	Cr(III) Adsorption by Cluster Formation on Boehmite Nanoplates in Highly Alkaline Solution. *Environmental Science & Technology*, **2019**, 53, 11043-11055	10.3	27
283	Cluster embedding of ionic systems: Point charges and extended ions. *Journal of Chemical Physics*, **2019**, 151, 044107	3.9	8

282	Unraveling Gibbsite Transformation Pathways into LiAl-LDH in Concentrated Lithium Hydroxide. *Inorganic Chemistry*, **2019**, 58, 12385-12394	5.1	10
281	Redistribution of Electron Equivalents between Magnetite and Aqueous Fe Induced by a Model Quinone Compound AQDS. *Environmental Science & Technology*, **2019**, 53, 1863-1873	10.3	11
280	Lateral water structure connects metal oxide nanoparticle faces. *Journal of Materials Research*, **2019**, 34, 456-464	2.5	2
279	Anomalously low activation energy of nanoconfined MgCO precipitation. *Chemical Communications*, **2019**, 55, 6835-6837	5.8	10
278	Surface-Catalyzed Oxygen Exchange during Mineral Carbonation in Nanoscale Water Films. *Journal of Physical Chemistry C*, **2019**,	3.8	12
277	Natural, incidental, and engineered nanomaterials and their impacts on the Earth system. *Science*, **2019**, 363,	33.3	250
276	Visualizing the iron atom exchange front in the Fe(II)-catalyzed recrystallization of goethite by atom probe tomography. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 2866-2874	11.5	34
275	Facet-Specific Photocatalytic Degradation of Organics by Heterogeneous Fenton Chemistry on Hematite Nanoparticles. *Environmental Science & Technology*, **2019**, 53, 10197-10207	10.3	57
274	Electron- and Thermal-Stimulated Synthesis of Water on Boehmite (AlOOH) Nanoplates. *Journal of Physical Chemistry C*, **2019**, 123, 18986-18992	3.8	5
273	Quantitative Review of Olivine Carbonation Kinetics: Reactivity Trends, Mechanistic Insights, and Research Frontiers. *Environmental Science and Technology Letters*, **2019**, 6, 431-442	11	16
272	Effect of structure and composition on the electronic excitation induced amorphization of LaTiZrO ceramics. *Scientific Reports*, **2019**, 9, 8190	4.9	4
271	Facet-selective adsorption of Fe(II) on hematite visualized by nanoscale secondary ion mass spectrometry. *Environmental Science: Nano*, **2019**, 6, 2429-2440	7.1	8
270	Reply to Comment on Roles of Hydration and Magnetism on the Structure of Ferrihydrite from First Principles *ACS Earth and Space Chemistry*, **2019**, 3, 1581-1583	3.2	3
269	Structure, Magnetism, and the Interaction of Water with Ti-Doped FeO Surfaces. *Langmuir*, **2019**, 35, 13872-13879	4	4
268	A Closer Look at Fe(II) Passivation of Goethite. *ACS Earth and Space Chemistry*, **2019**, 3, 2717-2725	3.2	9
267	Iron Redox Chemistry and Its Environmental Impact: A Virtual Special Issue. *ACS Earth and Space Chemistry*, **2019**, 3, 2374-2375	3.2	1
266	Synthesis of 2D Hexagonal Hematite Nanosheets and the Crystal Growth Mechanism. *Inorganic Chemistry*, **2019**, 58, 16727-16735	5.1	14
265	Reductive Dissolution Mechanisms at the Hematite-Electrolyte Interface Probed by in Situ X-ray Scattering. *Journal of Physical Chemistry C*, **2019**, 123, 8077-8085	3.8	6

264	Energetics and the Role of Defects in Fe(II)-Catalyzed Goethite Recrystallization from Molecular Simulations. *ACS Earth and Space Chemistry*, **2019**, 3, 262-272	3.2	11
263	Radiocesium interaction with clay minerals: Theory and simulation advances Post-Fukushima. *Journal of Environmental Radioactivity*, **2019**, 210, 105809	2.4	6
262	Roles of Hydration and Magnetism on the Structure of Ferrihydrite from First Principles. *ACS Earth and Space Chemistry*, **2019**, 3, 70-78	3.2	14
261	Radiocesium interaction with clay minerals: Theory and simulation advances Post-Fukushima. *Journal of Environmental Radioactivity*, **2018**, 189, 135-145	2.4	45
260	Surface Charge Effects on Fe(II) Sorption and Oxidation at (110) Goethite Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 10059-10066	3.8	6
259	Radiolytic stability of gibbsite and boehmite with adsorbed water. *Journal of Nuclear Materials*, **2018**, 501, 224-233	3.3	24
258	Electrochemical Interfaces: Potential-Specific Structure at the Hematite□Electrolyte Interface (Adv. Funct. Mater. 8/2018). *Advanced Functional Materials*, **2018**, 28, 1870054	15.6	1
257	Resolving Iron(II) Sorption and Oxidative Growth on Hematite (001) Using Atom Probe Tomography. *Journal of Physical Chemistry C*, **2018**, 122, 3903-3914	3.8	20
256	Synthesis of nanometer-sized fayalite and magnesium-iron(II) mixture olivines. *Journal of Colloid and Interface Science*, **2018**, 515, 129-138	9.3	14
255	The Role of Defects in Fe(II)-Goethite Electron Transfer. *Environmental Science & Technology*, **2018**, 52, 2751-2759	10.3	44
254	Consequences of realistic embedding for the L edge XAS of □FeO. *Physical Chemistry Chemical Physics*, **2018**, 20, 4396-4403	3.6	12
253	Size and Morphology Controlled Synthesis of Boehmite Nanoplates and Crystal Growth Mechanisms. *Crystal Growth and Design*, **2018**, 18, 3596-3606	3.5	58
252	Free-Energy Landscape of the Dissolution of Gibbsite at High pH. *Journal of Physical Chemistry Letters*, **2018**, 9, 1809-1814	6.4	14
251	In Situ Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions above and below Saturation with Respect to Gibbsite. *Inorganic Chemistry*, **2018**, 57, 11864-11873	5.1	23
250	Facet-dependent contaminant removal properties of hematite nanocrystals and their environmental implications. *Environmental Science: Nano*, **2018**, 5, 1790-1806	7.1	64
249	Technetium Stabilization in Low-Solubility Sulfide Phases: A Review. *ACS Earth and Space Chemistry*, **2018**, 2, 532-547	3.2	27
248	Water Structure Controls Carbonic Acid Formation in Adsorbed Water Films. *Journal of Physical Chemistry Letters*, **2018**, 9, 4988-4994	6.4	11
247	Reversible Fe(II) uptake/release by magnetite nanoparticles. *Environmental Science: Nano*, **2018**, 5, 1545-1555	7.1	13

246	Potential-Specific Structure at the Hematite□lectrolyte Interface. *Advanced Functional Materials*, **2018**, 28, 1705618	15.6	13
245	Al Pulsed Field Gradient, Diffusion-NMR Spectroscopy of Solvation Dynamics and Ion Pairing in Alkaline Aluminate Solutions. *Journal of Physical Chemistry B*, **2018**, 122, 10907-10912	3.4	11
244	Boehmite and Gibbsite Nanoplates for the Synthesis of Advanced Alumina Products. *ACS Applied Nano Materials*, **2018**, 1, 7115-7128	5.6	39
243	Effects of Ionic Strength, Salt, and pH on Aggregation of Boehmite Nanocrystals: Tumbler Small-Angle Neutron and X-ray Scattering and Imaging Analysis. *Langmuir*, **2018**, 34, 15839-15853	4	20
242	Acidity Constants of the Hematite-Liquid Water Interface from Ab Initio Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2018**, 9, 5574-5582	6.4	20
241	Impact of Solution Chemistry and Particle Anisotropy on the Collective Dynamics of Oriented Aggregation. *ACS Nano*, **2018**, 12, 10114-10122	16.7	28
240	X-ray Linear Dichroism in Apatite. *Journal of the American Chemical Society*, **2018**, 140, 11698-11704	16.4	14
239	Accessing crystal-crystal interaction forces with oriented nanocrystal atomic force microscopy probes. *Nature Protocols*, **2018**, 13, 2005-2030	18.8	9
238	Surface Chemistry Affects the Efficacy of the Hydration Force between Two ZnO(101 0) Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 12259-12266	3.8	15
237	First-Principles Investigation of Native Interstitial Diffusion in Cr2O3. *Journal of Physical Chemistry C*, **2018**, 122, 12984-12993	3.8	15
236	A Thermodynamic Model for ZrO2(am) Solubility at 25 □C in the Ca2+□Na+□H+□Cl□OH□H2O System: A Critical Review. *Journal of Solution Chemistry*, **2018**, 47, 855-891	1.8	4
235	Corresponding Orbitals Derived from Periodic Bloch States for Electron Transfer Calculations of Transition Metal Oxides. *Journal of Chemical Theory and Computation*, **2018**, 14, 4416-4426	6.4	11
234	Ab Initio Molecular Dynamics Reveal Spectroscopic Siblings and Ion Pairing as New Challenges for Elucidating Prenucleation Aluminum Speciation. *Journal of Physical Chemistry B*, **2018**, 122, 7394-7402	3.4	25
233	Iron Dissolution from Goethite (□FeOOH) Surfaces in Water by Ab Initio Enhanced Free-Energy Simulations. *Journal of Physical Chemistry C*, **2018**, 122, 16086-16091	3.8	19
232	Vacancies and Vacancy-Mediated Self Diffusion in Cr2O3: A First-Principles Study. *Journal of Physical Chemistry C*, **2017**, 121, 1817-1831	3.8	20
231	Dynamic Stabilization of Metal Oxide-Water Interfaces. *Journal of the American Chemical Society*, **2017**, 139, 2581-2584	16.4	48
230	Direction-specific van der Waals attraction between rutile TiO nanocrystals. *Science*, **2017**, 356, 434-437	33.3	80
229	Electron Mobility and Trapping in Ferrihydrite Nanoparticles. *ACS Earth and Space Chemistry*, **2017**, 1, 216-226	3.2	13

228	Stochastic Simulation of Isotopic Exchange Mechanisms for Fe(II)-Catalyzed Recrystallization of Goethite. *Environmental Science & Technology*, **2017**, 51, 7552-7559	10.3	17
227	Improving the Performance of Hybrid Functional-Based Molecular Dynamics Simulation through Screening of Hartree-Fock Exchange Forces. *Journal of Chemical Theory and Computation*, **2017**, 13, 2178-2184	5.4	7
226	Nucleation and Epitaxy-Mediated Phase Transformation of a Precursor Cadmium Carbonate Phase at the Calcite/Water Interface. *Journal of Physical Chemistry C*, **2017**, 121, 5012-5019	3.8	11
225	Water Solubility at Saturation for CO2□H4 Mixtures at 323.2 K and 9.000 MPa. *Journal of Chemical & Engineering Data*, **2017**, 62, 1608-1614	2.8	16
224	Direction-specific interaction forces underlying zinc oxide crystal growth by oriented attachment. *Nature Communications*, **2017**, 8, 835	17.4	64
223	Tipping Point for Expansion of Layered Aluminosilicates in Weakly Polar Solvents: Supercritical CO. *ACS Applied Materials & Interfaces*, **2017**, 9, 36783-36791	9.5	29
222	Transmutation effects on long-term Cs retention in phyllosilicate minerals from first principles. *Physical Chemistry Chemical Physics*, **2017**, 19, 27007-27014	3.6	4
221	Reply to □omments on Radiation-Damage Resistance in Phyllosilicate Minerals from First Principles and Implications for Radiocesium and Strontium Retention in Soils□*Clays and Clay Minerals*, **2017**, 65, 371-375	2.1	2
220	Impact of Ti Incorporation on Hydroxylation and Wetting of Fe3O4. *Journal of Physical Chemistry C*, **2017**, 121, 19288-19295	3.8	8
219	First-Principles Fe L-Edge and O K-Edge XANES and XMCD Spectra for Iron Oxides. *Journal of Physical Chemistry A*, **2017**, 121, 7613-7618	2.8	22
218	Mechanisms and Rates of U(VI) Reduction by Fe(II) in Homogeneous Aqueous Solution and the Role of U(V) Disproportionation. *Journal of Physical Chemistry A*, **2017**, 121, 6603-6613	2.8	13
217	Electron Transfer Pathways Facilitating U(VI) Reduction by Fe(II) on Al- vs Fe-Oxides. *Journal of Physical Chemistry C*, **2017**, 121, 19887-19903	3.8	13
216	Transitions in Al Coordination during Gibbsite Crystallization Using High-Field 27Al and 23Na MAS NMR Spectroscopy. *Journal of Physical Chemistry C*, **2017**, 121, 27555-27562	3.8	33
215	A thermodynamic model for the solubility of HfO2(am) in the aqueous K + □HCO3 □CO32 □ OH □H2O system. *Radiochimica Acta*, **2017**, 105, 637-647	1.9	1
214	Fast Synthesis of Gibbsite Nanoplates and Process Optimization using Box-Behnken Experimental Design. *Crystal Growth and Design*, **2017**, 17, 6801-6808	3.5	37
213	Redox potentials in the decaheme cytochrome MtrF: Poisson-Boltzmann vs. molecular dynamics simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E10028	11.5	2
212	Tc(VII) and Cr(VI) Interaction with Naturally Reduced Ferruginous Smectite from a Redox Transition Zone. *Environmental Science & Technology*, **2017**, 51, 9042-9052	10.3	26
211	Trends in mica-mica adhesion reflect the influence of molecular details on long-range dispersion forces underlying aggregation and coalignment. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 7537-7542	11.5	39

210	Probing size-dependent electrokinetics of hematite aggregates. *Journal of Colloid and Interface Science*, **2017**, 488, 218-224	9.3	8
209	Analysis of X-ray adsorption edges: L edge of FeCl. *Journal of Chemical Physics*, **2017**, 147, 224306	3.9	12
208	Origin of 6-fold coordinated aluminum at (010)-type pyrophyllite edges. *AIP Advances*, **2017**, 7, 055211	1.5	6
207	Hematite(001)-liquid water interface from hybrid density functional-based molecular dynamics. *Journal of Physics Condensed Matter*, **2016**, 28, 394001	1.8	17
206	Particle size effect and the mechanism of hematite reduction by the outer membrane cytochrome OmcA of Shewanella oneidensis MR-1. *Geochimica Et Cosmochimica Acta*, **2016**, 193, 160-175	5.5	28
205	The origin of facet selectivity and alignment in anatase TiO nanoparticles in electrolyte solutions: implications for oriented attachment in metal oxides. *Nanoscale*, **2016**, 8, 19714-19725	7.7	37
204	Adsorption and diffusion of atomic oxygen and sulfur at pristine and doped Ni surfaces with implications for stress corrosion cracking. *Corrosion Science*, **2016**, 113, 26-30	6.8	11
203	In Situ Natural Abundance O and Mg NMR Investigation of Aqueous Mg(OH) Dissolution in the Presence of Supercritical CO. *Environmental Science & Technology*, **2016**, 50, 12373-12384	10.3	5
202	Size dependent microbial oxidation and reduction of magnetite nano- and micro-particles. *Scientific Reports*, **2016**, 6, 30969	4.9	23
201	Issues concerning the determination of solubility products of sparingly soluble crystalline solids: solubility of HfO2(cr). *Radiochimica Acta*, **2016**, 104, 583-592	1.9	3
200	An X-ray magnetic circular dichroism (XMCD) study of Fe ordering in a synthetic MgAl2O4-Fe3O4 (spinel-magnetite) solid-solution series: Implications for magnetic properties and cation site ordering. *American Mineralogist*, **2016**, 101, 1373-1388	2.9	7
199	Fast Interconversion of Hydrogen Bonding at the Hematite (001)-Liquid Water Interface. *Journal of Physical Chemistry Letters*, **2016**, 7, 1155-60	6.4	30
198	Radiation-Damage Resistance in Phyllosilicate Minerals from First Principles and Implications for Radiocesium and Strontium Retention in Soils. *Clays and Clay Minerals*, **2016**, 64, 108-114	2.1	6
197	Molecular Simulation of Cesium Adsorption at the Basal Surface of Phyllosilicate Minerals. *Clays and Clay Minerals*, **2016**, 64, 389-400	2.1	23
196	An in situ XAS study of ferric iron hydrolysis and precipitation in the presence of perchlorate, nitrate, chloride and sulfate. *Geochimica Et Cosmochimica Acta*, **2016**, 177, 150-169	5.5	21
195	Geochemical Kinetics via Computational Chemistry **2016**, 375-414		1
194	Intermediate coupling for core-level excited states: Consequences for X-Ray absorption spectroscopy. *Journal of Electron Spectroscopy and Related Phenomena*, **2015**, 200, 174-180	1.7	12
193	Evidence for Carbonate Surface Complexation during Forsterite Carbonation in Wet Supercritical Carbon Dioxide. *Langmuir*, **2015**, 31, 7533-43	4	36

192	Multiscale model of metal alloy oxidation at grain boundaries. *Journal of Chemical Physics*, **2015**, 142, 214114	3.9	7
191	Iron Atom Exchange between Hematite and Aqueous Fe(II). *Environmental Science & Technology*, **2015**, 49, 8479-86	10.3	69
190	Low temperature, non-stoichiometric oxygen-isotope exchange coupled to Fe(II)-goethite interactions. *Geochimica Et Cosmochimica Acta*, **2015**, 160, 38-54	5.5	22
189	Ab Initio Modeling of Bulk and Intragranular Diffusion in Ni Alloys. *Journal of Physical Chemistry Letters*, **2015**, 6, 1618-23	6.4	20
188	Role of hydration forces in the properties of electrolyte solutions in the bulk and at interfaces. *Materials Research Society Symposia Proceedings*, **2015**, 1753, 38		1
187	Modeling selective intergranular oxidation of binary alloys. *Journal of Chemical Physics*, **2015**, 142, 014704	3.9	2
186	Redox cycling of Fe(II) and Fe(III) in magnetite by Fe-metabolizing bacteria. *Science*, **2015**, 347, 1473-6	33.3	160
185	Ab initio modeling of Fe(II) adsorption and interfacial electron transfer at goethite (α-FeOOH) surfaces. *Physical Chemistry Chemical Physics*, **2015**, 17, 14518-31	3.6	48
184	Proton Dynamics on Goethite Nanoparticles and Coupling to Electron Transport. *Journal of Chemical Theory and Computation*, **2015**, 11, 1715-24	6.4	13
183	Computational Molecular Simulation of the Oxidative Adsorption of Ferrous Iron at the Hematite (001)-Water Interface. *Journal of Physical Chemistry C*, **2015**, 119, 9242-9252	3.8	25
182	Potentiometric and electrokinetic signatures of iron(II) interactions with (α)-Fe2O3. *Physical Chemistry Chemical Physics*, **2015**, 17, 26264-9	3.6	3
181	Dynamics of Magnesite Formation at Low Temperature and High pCO2 in Aqueous Solution. *Environmental Science & Technology*, **2015**, 49, 10736-44	10.3	16
180	Multi-haem cytochromes in Shewanella oneidensis MR-1: structures, functions and opportunities. *Journal of the Royal Society Interface*, **2015**, 12, 20141117	4.1	146
179	Spontaneous water oxidation at hematite (α-Fe2O3) crystal faces. *ACS Applied Materials & Interfaces*, **2015**, 7, 1550-9	9.5	29
178	Capturing ultrafast photoinduced local structural distortions of BiFeO3. *Scientific Reports*, **2015**, 5, 15098	4.9	18
177	Flavin Binding to the Deca-heme Cytochrome MtrC: Insights from Computational Molecular Simulation. *Biophysical Journal*, **2015**, 109, 2614-2624	2.9	12
176	Characterizing mineralogy and redox reactivity in potential host rocks for a UK geological disposal facility. *Mineralogical Magazine*, **2015**, 79, 1353-1367	1.7	5
175	Heterogeneous growth of cadmium and cobalt carbonate phases at the 10-14 calcite surface. *Chemical Geology*, **2015**, 397, 24-36	4.2	14

174	Charge Transport at Ti-Doped Hematite (001)/Aqueous Interfaces. *Chemistry of Materials*, **2015**, 27, 1665-1673	9.466	23
173	Atom exchange between aqueous Fe(II) and structural Fe in clay minerals. *Environmental Science & Technology*, **2015**, 49, 2786-95	10.3	30
172	Molecular Dynamics Study of Fe(II) Adsorption, Electron Exchange, and Mobility at Goethite (□FeOOH) Surfaces. *Journal of Physical Chemistry C*, **2015**, 119, 3111-3123	3.8	51
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