

# Kevin M Rosso

## List of Publications by Citations

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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	Electrically conductive bacterial nanowires produced by <i>Shewanella oneidensis</i> strain MR-1 and other microorganisms. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2006</b> , 103, 11358-63	11.5	1359
334	Nanostructures and lithium electrochemical reactivity of lithium titanites and titanium oxides: A review. <i>Journal of Power Sources</i> , <b>2009</b> , 192, 588-598	8.9	717
333	Linked reactivity at mineral-water interfaces through bulk crystal conduction. <i>Science</i> , <b>2008</b> , 320, 218-223	33.3	277
332	Role of extracellular polymeric substances in bioflocculation of activated sludge microorganisms under glucose-controlled conditions. <i>Water Research</i> , <b>2010</b> , 44, 4505-16	12.5	275
331	Charge transport in metal oxides: a theoretical study of hematite $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> . <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 144305	3.9	253
330	Natural, incidental, and engineered nanomaterials and their impacts on the Earth system. <i>Science</i> , <b>2019</b> , 363,	33.3	250
329	An ab initio model of electron transport in hematite ( $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> ) basal planes. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 6455-6466	3.9	247
328	The roles of outer membrane cytochromes of <i>Shewanella</i> and <i>Geobacter</i> in extracellular electron transfer. <i>Environmental Microbiology Reports</i> , <b>2009</b> , 1, 220-7	3.7	236
327	Redox cycling of Fe(II) and Fe(III) in magnetite by Fe-metabolizing bacteria. <i>Science</i> , <b>2015</b> , 347, 1473-6	33.3	160
326	Multi-haem cytochromes in <i>Shewanella oneidensis</i> MR-1: structures, functions and opportunities. <i>Journal of the Royal Society Interface</i> , <b>2015</b> , 12, 20141117	4.1	146
325	Molecular Underpinnings of Fe(III) Oxide Reduction by <i>Shewanella Oneidensis</i> MR-1. <i>Frontiers in Microbiology</i> , <b>2012</b> , 3, 50	5.7	141
324	Electron flow in multiheme bacterial cytochromes is a balancing act between heme electronic interaction and redox potentials. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2014</b> , 111, 611-6	11.5	136
323	Electron small polarons and their mobility in iron (oxyhydr)oxide nanoparticles. <i>Science</i> , <b>2012</b> , 337, 1200-3	33.3	136
322	A trans-outer membrane porin-cytochrome protein complex for extracellular electron transfer by <i>Geobacter sulfurreducens</i> PCA. <i>Environmental Microbiology Reports</i> , <b>2014</b> , 6, 776-85	3.7	130
321	Identification and Characterization of MtoA: A Decaheme c-Type Cytochrome of the Neutrophilic Fe(II)-Oxidizing Bacterium <i>Sideroxydans lithotrophicus</i> ES-1. <i>Frontiers in Microbiology</i> , <b>2012</b> , 3, 37	5.7	130
320	In situ infrared spectroscopic study of forsterite carbonation in wet supercritical CO <sub>2</sub> . <i>Environmental Science &amp; Technology</i> , <b>2011</b> , 45, 6204-10	10.3	127
319	The structure of hematite ( $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> ) (001) surfaces in aqueous media: scanning tunneling microscopy and resonant tunneling calculations of coexisting O and Fe terminations. <i>Geochimica Et Cosmochimica Acta</i> , <b>2003</b> , 67, 985-1000	5.5	121

318	Fe(II)-catalyzed recrystallization of goethite revisited. <i>Environmental Science &amp; Technology</i> , <b>2014</b> , 48, 11302-11	10.3	114
317	Ab Initio Determination of Edge Surface Structures for Dioctahedral 2:1 Phyllosilicates: Implications for Acid-Base Reactivity. <i>Clays and Clay Minerals</i> , <b>2003</b> , 51, 359-371	2.1	113
316	The interaction of pyrite {100} surfaces with O <sub>2</sub> and H <sub>2</sub> O: Fundamental oxidation mechanisms. <i>American Mineralogist</i> , <b>1999</b> , 84, 1549-1561	2.9	108
315	In situ molecular spectroscopic evidence for CO <sub>2</sub> intercalation into montmorillonite in supercritical carbon dioxide. <i>Langmuir</i> , <b>2012</b> , 28, 7125-8	4	107
314	Bond-valence methods for pK <sub>a</sub> prediction: critical reanalysis and a new approach. <i>Geochimica Et Cosmochimica Acta</i> , <b>2004</b> , 68, 2025-2042	5.5	105
313	The proximity effect on semiconducting mineral surfaces: a new aspect of mineral surface reactivity and surface complexation theory?. <i>Geochimica Et Cosmochimica Acta</i> , <b>2001</b> , 65, 2641-2649	5.5	105
312	Mtr extracellular electron-transfer pathways in Fe(III)-reducing or Fe(II)-oxidizing bacteria: a genomic perspective. <i>Biochemical Society Transactions</i> , <b>2012</b> , 40, 1261-7	5.1	103
311	Influence of dynamical conditions on the reduction of U(VI) at the magnetite-solution interface. <i>Environmental Science &amp; Technology</i> , <b>2010</b> , 44, 170-6	10.3	100
310	Atomically resolved electronic structure of pyrite {100} surfaces; an experimental and theoretical investigation with implications for reactivity. <i>American Mineralogist</i> , <b>1999</b> , 84, 1535-1548	2.9	98
309	Connecting observations of hematite (alpha-Fe <sub>2</sub> O <sub>3</sub> ) growth catalyzed by Fe(II). <i>Environmental Science &amp; Technology</i> , <b>2010</b> , 44, 61-7	10.3	97
308	Spectroscopic characterization of extracellular polymeric substances from Escherichia coli and Serratia marcescens: suppression using sub-inhibitory concentrations of bismuth thiols. <i>Biomacromolecules</i> , <b>2008</b> , 9, 3079-89	6.9	94
307	Combined 6,7Li NMR and Molecular Dynamics Study of Li Diffusion in Li <sub>2</sub> TiO <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 20108-20116	3.8	91
306	Nonlocal bacterial electron transfer to hematite surfaces. <i>Geochimica Et Cosmochimica Acta</i> , <b>2003</b> , 67, 1081-1087	5.5	89
305	The role of H <sub>2</sub> O in the carbonation of forsterite in supercritical CO <sub>2</sub> . <i>International Journal of Greenhouse Gas Control</i> , <b>2011</b> , 5, 1081-1092	4.2	84
304	CO <sub>2</sub> sorption to subsingle hydration layer montmorillonite clay studied by excess sorption and neutron diffraction measurements. <i>Environmental Science &amp; Technology</i> , <b>2013</b> , 47, 205-11	10.3	83
303	In situ study of CO <sub>2</sub> and H <sub>2</sub> O partitioning between Na-montmorillonite and variably wet supercritical carbon dioxide. <i>Langmuir</i> , <b>2014</b> , 30, 6120-8	4	82
302	In situ X-ray diffraction study of Na <sup>+</sup> saturated montmorillonite exposed to variably wet supercritical CO <sub>2</sub> . <i>Environmental Science &amp; Technology</i> , <b>2012</b> , 46, 4241-8	10.3	82
301	Reaction of water-saturated supercritical CO <sub>2</sub> with forsterite: Evidence for magnesite formation at low temperatures. <i>Geochimica Et Cosmochimica Acta</i> , <b>2012</b> , 91, 271-282	5.5	81

300	Direction-specific van der Waals attraction between rutile TiO nanocrystals. <i>Science</i> , <b>2017</b> , 356, 434-437	33.3	80
299	Metal Carbonation of Forsterite in Supercritical CO <sub>2</sub> and H <sub>2</sub> O Using Solid State <sup>29</sup> Si, <sup>13</sup> C NMR Spectroscopy. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 4126-4134	3.8	79
298	Kinetics of reduction of Fe(III) complexes by outer membrane cytochromes MtrC and OmcA of <i>Shewanella oneidensis</i> MR-1. <i>Applied and Environmental Microbiology</i> , <b>2008</b> , 74, 6746-55	4.8	77
297	U(VI) sorption and reduction kinetics on the magnetite (111) surface. <i>Environmental Science &amp; Technology</i> , <b>2012</b> , 46, 3821-30	10.3	71
296	Computer simulation of electron transfer at hematite surfaces. <i>Geochimica Et Cosmochimica Acta</i> , <b>2006</b> , 70, 1888-1903	5.5	71
295	Iron Atom Exchange between Hematite and Aqueous Fe(II). <i>Environmental Science &amp; Technology</i> , <b>2015</b> , 49, 8479-86	10.3	69
294	Thermodynamics of electron flow in the bacterial deca-heme cytochrome MtrF. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 9868-71	16.4	68
293	Mechanism of Li <sup>+</sup> /Electron Conductivity in Rutile and Anatase TiO <sub>2</sub> Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 20277-20283	3.8	68
292	Structure and oxidation state of hematite surfaces reacted with aqueous Fe(II) at acidic and neutral pH. <i>Geochimica Et Cosmochimica Acta</i> , <b>2010</b> , 74, 1498-1512	5.5	68
291	Surface structure effects on direct reduction of iron oxides by <i>Shewanella oneidensis</i> . <i>Geochimica Et Cosmochimica Acta</i> , <b>2003</b> , 67, 4489-4503	5.5	68
290	Synthesis and properties of titanomagnetite (Fe <sub>3-x</sub> Ti <sub>x</sub> O <sub>4</sub> ) nanoparticles: a tunable solid-state Fe(II/III) redox system. <i>Journal of Colloid and Interface Science</i> , <b>2012</b> , 387, 24-38	9.3	65
289	Direction-specific interaction forces underlying zinc oxide crystal growth by oriented attachment. <i>Nature Communications</i> , <b>2017</b> , 8, 835	17.4	64
288	Facet-dependent contaminant removal properties of hematite nanocrystals and their environmental implications. <i>Environmental Science: Nano</i> , <b>2018</b> , 5, 1790-1806	7.1	64
287	Surface potentials of (001), (012), (113) hematite (Fe <sub>2</sub> O <sub>3</sub> ) crystal faces in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 13911-21	3.6	63
286	Forsterite [Mg <sub>2</sub> SiO <sub>4</sub> ] carbonation in wet supercritical CO <sub>2</sub> : an in situ high-pressure X-ray diffraction study. <i>Environmental Science &amp; Technology</i> , <b>2013</b> , 47, 174-81	10.3	63
285	Bond-valence methods for pK <sub>a</sub> prediction. II. Bond-valence, electrostatic, molecular geometry, and solvation effects. <i>Geochimica Et Cosmochimica Acta</i> , <b>2006</b> , 70, 4057-4071	5.5	60
284	Molecular Computational Investigation of Electron-Transfer Kinetics Across Cytochrome Iron Oxide Interfaces. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 11363-11375	3.8	59
283	Size and Morphology Controlled Synthesis of Boehmite Nanoplates and Crystal Growth Mechanisms. <i>Crystal Growth and Design</i> , <b>2018</b> , 18, 3596-3606	3.5	58

282	Molecular Dynamics Characterization of Rutile-Anatase Interfaces. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 9290-9298	3.8	58
281	Outer-sphere electron transfer kinetics of metal ion oxidation by molecular oxygen. <i>Geochimica Et Cosmochimica Acta</i> , <b>2002</b> , 66, 4223-4233	5.5	58
280	Ab Initio Calculation of Homogeneous Outer Sphere Electron Transfer Rates: Application to M(OH <sub>2</sub> ) <sub>6</sub> <sup>3+</sup> /2+ Redox Couples. <i>Journal of Physical Chemistry A</i> , <b>2000</b> , 104, 6718-6725	2.8	58
279	Facet-Specific Photocatalytic Degradation of Organics by Heterogeneous Fenton Chemistry on Hematite Nanoparticles. <i>Environmental Science &amp; Technology</i> , <b>2019</b> , 53, 10197-10207	10.3	57
278	Kinetic Monte Carlo model of charge transport in hematite (alpha-Fe(2)O(3)). <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 124706	3.9	56
277	Oxygen Vacancies and Ordering of d-levels Control Voltage Suppression in Oxide Cathodes: the Case of Spinel LiNi <sub>0.5</sub> Mn <sub>1.5</sub> O <sub>4</sub> . <i>Advanced Functional Materials</i> , <b>2013</b> , 23, 5530-5535	15.6	55
276	Electron transfer in environmental systems: a frontier for theoretical chemistry. <i>Theoretical Chemistry Accounts</i> , <b>2006</b> , 116, 124-136	1.9	54
275	Charge and Ion Transport in NiO and Aspects of Ni Oxidation from First Principles. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 1948-1954	3.8	53
274	Structure, charge distribution, and electron hopping dynamics in magnetite (Fe <sub>3</sub> O <sub>4</sub> ) (100) surfaces from first principles. <i>Geochimica Et Cosmochimica Acta</i> , <b>2010</b> , 74, 4234-4248	5.5	53
273	Electron tunneling properties of outer-membrane decaheme cytochromes from <i>Shewanella oneidensis</i> . <i>Geochimica Et Cosmochimica Acta</i> , <b>2007</b> , 71, 543-555	5.5	52
272	Electron density distribution and bond critical point properties for forsterite, Mg <sub>2</sub> SiO <sub>4</sub> , determined with synchrotron single crystal X-ray diffraction data. <i>Physics and Chemistry of Minerals</i> , <b>2005</b> , 32, 301-313	1.6	52
271	Molecular Dynamics Study of Fe(II) Adsorption, Electron Exchange, and Mobility at Goethite (FeOOH) Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 3111-3123	3.8	51
270	Effect of Chemical Lithium Insertion into Rutile TiO <sub>2</sub> Nanorods. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 14567-14574	3.8	51
269	Bismuth dimercaptopropanol (BisBAL) inhibits the expression of extracellular polysaccharides and proteins by <i>Brevundimonas diminuta</i> : implications for membrane microfiltration. <i>Biotechnology and Bioengineering</i> , <b>2008</b> , 99, 634-43	4.9	51
268	In situ infrared spectroscopic study of brucite carbonation in dry to water-saturated supercritical carbon dioxide. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 4768-77	2.8	50
267	Lithium diffusion in Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> at high temperatures. <i>Journal of Power Sources</i> , <b>2011</b> , 196, 2211-2220	8.9	50
266	Identification of simultaneous U(VI) sorption complexes and U(IV) nanoprecipitates on the magnetite (111) surface. <i>Environmental Science &amp; Technology</i> , <b>2012</b> , 46, 3811-20	10.3	49
265	Mechanisms of electron transfer in two decaheme cytochromes from a metal-reducing bacterium. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 12857-64	3.4	49

- 264 Dynamic Stabilization of Metal Oxide-Water Interfaces. *Journal of the American Chemical Society*, **2017**, 139, 2581-2584 16.4 48
- 263 Ab initio modeling of Fe(II) adsorption and interfacial electron transfer at goethite (FeOOH) surfaces. *Physical Chemistry Chemical Physics*, **2015**, 17, 14518-31 3.6 48
- 262 Structure and Charge Hopping Dynamics in Green Rust. *Journal of Physical Chemistry C*, **2007**, 111, 11414-11423 3.8 48
- 261 Metal oxidation kinetics and the transition from thin to thick films. *Physical Chemistry Chemical Physics*, **2012**, 14, 14534-9 3.6 47
- 260 A Shell Model for Atomistic Simulation of Charge Transfer in Titania. *Journal of Physical Chemistry C*, **2008**, 112, 7678-7688 3.8 46
- 259 Reactivity of Sulfide Mineral Surfaces. *Reviews in Mineralogy and Geochemistry*, **2006**, 61, 557-607 7.1 46
- 258 Radiocesium interaction with clay minerals: Theory and simulation advances Post-Fukushima. *Journal of Environmental Radioactivity*, **2018**, 189, 135-145 2.4 45
- 257 The Role of Defects in Fe(II)-Goethite Electron Transfer. *Environmental Science & Technology*, **2018**, 52, 2751-2759 10.3 44
- 256 Insights into the Mechanism of Fe(II) Adsorption and Oxidation at Fe(II) Clay Mineral Surfaces from First-Principles Calculations. *Journal of Physical Chemistry C*, **2013**, 117, 22880-22886 3.8 44
- 255 Dynamics of Coupled Lithium/Electron Diffusion in TiO<sub>2</sub> Polymorphs. *Journal of Physical Chemistry C*, **2009**, 113, 20998-21007 3.8 44
- 254 Reorganization energy associated with small polaron mobility in iron oxide. *Journal of Chemical Physics*, **2004**, 120, 7050-4 3.9 44
- 253 Technetium incorporation into hematite (alpha-Fe<sub>2</sub>O<sub>3</sub>). *Environmental Science & Technology*, **2010**, 44, 5855-61 10.3 43
- 252 Electronic coupling between heme electron-transfer centers and its decay with distance depends strongly on relative orientation. *Journal of Physical Chemistry B*, **2006**, 110, 15582-8 3.4 42
- 251 Adatom Fe(III) on the hematite surface: Observation of a key reactive surface species. *Geochemical Transactions*, **2004**, 5, 1 3 42
- 250 Self-Exchange Electron Transfer Kinetics and Reduction Potentials for Anthraquinone Disulfonate. *Journal of Physical Chemistry A*, **2004**, 108, 3292-3303 2.8 42
- 249 Shared and closed-shell O-O interactions in silicates. *Journal of Physical Chemistry A*, **2008**, 112, 3693-9 2.8 41
- 248 A comparison of procrystal and ab initio model representations of the electron-density distributions of minerals. *Physics and Chemistry of Minerals*, **2002**, 29, 369-385 1.6 41
- 247 Structures and energies of ALOOH and FeOOH polymorphs from plane wave pseudopotential calculations. *American Mineralogist*, **2001**, 86, 312-317 2.9 41



246	Computer simulation of the light yield nonlinearity of inorganic scintillators. <i>Journal of Applied Physics</i> , <b>2009</b> , 105, 114915	2.5	40
245	Reversible ketone hydrogenation and dehydrogenation for aqueous organic redox flow batteries. <i>Science</i> , <b>2021</b> , 372, 836-840	33.3	40
244	Trends in mica-mica adhesion reflect the influence of molecular details on long-range dispersion forces underlying aggregation and coalignment. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2017</b> , 114, 7537-7542	11.5	39
243	Comparative reactivity study of forsterite and antigorite in wet supercritical CO <sub>2</sub> by in situ infrared spectroscopy. <i>International Journal of Greenhouse Gas Control</i> , <b>2013</b> , 18, 246-255	4.2	39
242	Simple kinetic Monte Carlo models for dissolution pitting induced by crystal defects. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 204106	3.9	39
241	Electron density distributions calculated for the nickel sulfides millerite, vaesite, and heazlewoodite and nickel metal: a case for the importance of ni-ni bond paths for electron transport. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 21788-95	3.4	39
240	Boehmite and Gibbsite Nanoplates for the Synthesis of Advanced Alumina Products. <i>ACS Applied Nano Materials</i> , <b>2018</b> , 1, 7115-7128	5.6	39
239	The origin of facet selectivity and alignment in anatase TiO <sub>2</sub> nanoparticles in electrolyte solutions: implications for oriented attachment in metal oxides. <i>Nanoscale</i> , <b>2016</b> , 8, 19714-19725	7.7	37
238	Fast Synthesis of Gibbsite Nanoplates and Process Optimization using Box-Behnken Experimental Design. <i>Crystal Growth and Design</i> , <b>2017</b> , 17, 6801-6808	3.5	37
237	Charge transfer in FeO: a combined molecular-dynamics and ab initio study. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 224712	3.9	37
236	Charge transport in micas: The kinetics of FeII/III electron transfer in the octahedral sheet. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 9207-9218	3.9	37
235	Fe(II) Redox Chemistry in the Environment. <i>Chemical Reviews</i> , <b>2021</b> , 121, 8161-8233	68.1	37
234	Evidence for Carbonate Surface Complexation during Forsterite Carbonation in Wet Supercritical Carbon Dioxide. <i>Langmuir</i> , <b>2015</b> , 31, 7533-43	4	36
233	Clay Hydration/dehydration in Dry to Water-saturated Supercritical CO <sub>2</sub> : Implications for Caprock Integrity. <i>Energy Procedia</i> , <b>2013</b> , 37, 5443-5448	2.3	36
232	Kinetic Monte Carlo Study of Ambipolar Lithium Ion and Electron Polarons Diffusion into Nanostructured TiO <sub>2</sub> . <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 2076-2081	6.4	36
231	Thermodynamics of the magnetite-ulvöspinel (Fe <sub>3</sub> O <sub>4</sub> -Fe <sub>2</sub> TiO <sub>4</sub> ) solid solution. <i>American Mineralogist</i> , <b>2012</b> , 97, 1330-1338	2.9	36
230	Fe(3-x)Ti(x)O <sub>4</sub> nanoparticles as tunable probes of microbial metal oxidation. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 8896-907	16.4	36
229	Electron Exchange and Conduction in Nontronite from First-Principles. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 2032-2040	3.8	36

228	Chromium(III) Hydroxide Solubility in the Aqueous $K^+-H^+-OHECO_2-HCO_3^-CO_2H-H_2O$ System: A Thermodynamic Model. <i>Journal of Solution Chemistry</i> , <b>2007</b> , 36, 1261-1285	1.8	36
227	Effect of surface site interactions on potentiometric titration of hematite ( $Fe_2O_3$ ) crystal faces. <i>Journal of Colloid and Interface Science</i> , <b>2013</b> , 391, 125-34	9.3	35
226	Heterogeneous reduction of $PuO_2$ with Fe(II): importance of the Fe(III) reaction product. <i>Environmental Science &amp; Technology</i> , <b>2011</b> , 45, 3952-8	10.3	35
225	Proximity effects on semiconducting mineral surfaces II: Distance dependence of indirect interactions. <i>Geochimica Et Cosmochimica Acta</i> , <b>2003</b> , 67, 941-953	5.5	35
224	Visualizing the iron atom exchange front in the Fe(II)-catalyzed recrystallization of goethite by atom probe tomography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2019</b> , 116, 2866-2874	11.5	34
223	Electron transport in pure and substituted iron oxyhydroxides by small-polaron migration. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 234701	3.9	34
222	Kinetics of triscarbonato uranyl reduction by aqueous ferrous iron: a theoretical study. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 9691-701	2.8	34
221	Molecular dynamics investigation of ferrous-ferric electron transfer in a hydrolyzing aqueous solution: calculation of the pH dependence of the diabatic transfer barrier and the potential of mean force. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 7607-15	3.9	34
220	Transitions in Al Coordination during Gibbsite Crystallization Using High-Field $^{27}Al$ and $^{23}Na$ MAS NMR Spectroscopy. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 27555-27562	3.8	33
219	Inner-Helmholtz potential development at the hematite ( $Fe_2O_3$ ) (0 0 1) surface. <i>Geochimica Et Cosmochimica Acta</i> , <b>2011</b> , 75, 4113-4124	5.5	33
218	Size Effects on $Li^+$ /Electron Conductivity in $TiO_2$ Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , <b>2010</b> , 1, 1967-1972	6.4	33
217	Self-similar mesocrystals form via interface-driven nucleation and assembly. <i>Nature</i> , <b>2021</b> , 590, 416-422	50.4	33
216	Molecular structure and free energy landscape for electron transport in the decahaem cytochrome MtrF. <i>Biochemical Society Transactions</i> , <b>2012</b> , 40, 1198-203	5.1	32
215	The effect of pH and time on the extractability and speciation of uranium(VI) sorbed to $SiO_2$ . <i>Environmental Science &amp; Technology</i> , <b>2012</b> , 46, 6604-11	10.3	32
214	Experimental bond critical point and local energy density properties determined for Mn-O, Fe-O, and Co-O bonded interactions for tephroite, $Mn_2SiO_4$ , fayalite, $Fe_2SiO_4$ , and $Co_2SiO_4$ olivine and selected organic metal complexes: comparison with properties calculated for non-transition and transition metal M-O bonded interactions for silicates and oxides. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 7643-7645	2.8	32
213	A Connection between Empirical Bond Strength and the Localization of the Electron Density at the Bond Critical Points of the SiO Bonds in Silicates. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 7643-7645	2.8	32
212	Bond length and local energy density property connections for non-transition-metal oxide-bonded interactions. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 12259-66	2.8	31
211	The Cs/K exchange in muscovite interlayers: An Ab Initio treatment. <i>Clays and Clay Minerals</i> , <b>2001</b> , 49, 500-513	2.1	31



210	Fast Interconversion of Hydrogen Bonding at the Hematite (001)-Liquid Water Interface. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 1155-60	6.4	30
209	Atom exchange between aqueous Fe(II) and structural Fe in clay minerals. <i>Environmental Science &amp; Technology</i> , <b>2015</b> , 49, 2786-95	10.3	30
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58	Crystallization and Phase Transformations of Aluminum (Oxy)hydroxide Polymorphs in Caustic Aqueous Solution. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 9820-9832	5.1	6
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55	Radiocesium interaction with clay minerals: Theory and simulation advances Post-Fukushima. <i>Journal of Environmental Radioactivity</i> , <b>2019</b> , 210, 105809	2.4	6
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