Kevin M Rosso

List of Publications by Year
in descending order

346 papers	17,635 citations	16411 64 h-index	21474 114 g-index
356 all docs	356 docs citations	356 times ranked	15582 citing authors

#	Article	IF	Citations
1	²⁷Al NMR diffusometry of Al₁₃ Keggin nanoclusters. Magnetic Resonance in Chemistry, 2022, 60, 226-238.	1.1	3
2	In situ imaging of amorphous intermediates during brucite carbonation in supercritical CO2. Nature Materials, 2022, 21, 345-351.	13.3	18
3	The effect of Cr alloying on defect migration at Ni grain boundaries. Journal of Materials Science, 2022, 57, 10499-10516.	1.7	5
4	Understanding Competitive Phosphate and Silicate Adsorption on Goethite by Connecting Batch Experiments with Density Functional Theory Calculations. Environmental Science & Technology, 2022, 56, 823-834.	4.6	22
5	Origin of the complex main and satellite features in Fe 2p XPS of Fe₂O₃. Physical Chemistry Chemical Physics, 2022, 24, 4562-4575.	1.3	26
6	Electron-Stimulated Formation and Release of Molecular Hydrogen and Oxygen from Boehmite Nanoplatelet Films. Journal of Physical Chemistry C, 2022, 126, 2542-2547.	1.5	2
7	Understanding the Importance of Labile Fe(III) during Fe(II)-Catalyzed Transformation of Metastable Iron Oxyhydroxides. Environmental Science & Technology, 2022, 56, 3801-3811.	4.6	25
8	Ab Initio Evaluation of Solid-State Transformation Pathways from Ferrihydrite to Goethite. ACS Earth and Space Chemistry, 2022, 6, 800-809.	1.2	4
9	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.	3.3	9
10	Electron and Hole Mobilities in Bulk Hematite from Spin-Constrained Density Functional Theory. Journal of the American Chemical Society, 2022, 144, 4623-4632.	6.6	22
11	Radiolysis and Radiation-Driven Dynamics of Boehmite Dissolution Observed by In Situ Liquid-Phase TEM. Environmental Science & Technology, 2022, 56, 5029-5036.	4.6	8
12	pH dependent reactivity of boehmite surfaces from first principles molecular dynamics. Physical Chemistry Chemical Physics, 2022, 24, 14177-14186.	1.3	4
13	Implementation and Validation of Constrained Density Functional Theory Forces in the CP2K Package. Journal of Chemical Theory and Computation, 2022, 18, 4438-4446.	2.3	5
14	Hydroxide promotes ion pairing in the NaNO₂â€“NaOHâ€“H₂O system. Physical Chemistry Chemical Physics, 2021, 23, 112-122.	1.3	8
15	Facet-Dependent Photodegradation of Methylene Blue by Hematite Nanoplates in Visible Light. Environmental Science & Technology, 2021, 55, 677-688.	4.6	67
16	Self-similar mesocrystals form via interface-driven nucleation and assembly. Nature, 2021, 590, 416-422.	13.7	98
17	Predicting the temperature dependence of self-diffusion behavior in Ni-Cr alloys via molecular dynamics. Materials Today Communications, 2021, 26, 101982.	0.9	3
18	Combined multiplet theory and experiment for the Fe 2p and 3p XPS of FeO and Fe2O3. Journal of Chemical Physics, 2021, 154, 094709.	1.2	78

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19	Direct visualization of radiation-induced transformations at alkali halideâ€“air interfaces. Communications Chemistry, 2021, 4, .	2.0	2
20	The Steady March toward Biomimetic Nanoelectronics. ACS Nano, 2021, 15, 7844-7847.	7.3	2
21	Reversible ketone hydrogenation and dehydrogenation for aqueous organic redox flow batteries. Science, 2021, 372, 836-840.	6.0	135
22	Comments on the Theory of Complex XPS Spectra: Extracting Chemical Information from the Fe 3p XPS of Fe Oxides. Comments on Inorganic Chemistry, 2021, 41, 373-397.	3.0	8
23	Crystallization and Phase Transformations of Aluminum (Oxy)hydroxide Polymorphs in Caustic Aqueous Solution. Inorganic Chemistry, 2021, 60, 9820-9832.	1.9	15
24	Fe(II) Redox Chemistry in the Environment. Chemical Reviews, 2021, 121, 8161-8233.	23.0	242
25	Synergistic Coupling of CO₂ and H₂O during Expansion of Clays in Supercritical CO₂â€“CH₄ Fluid Mixtures. Environmental Science & Technology, 2021, 55, 11192-11203.	4.6	3
26	Ab initio thermodynamics reveals the nanocomposite structure of ferrihydrite. Communications Chemistry, 2021, 4, .	2.0	17
27	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.	1.6	24
28	Cluster defects in gibbsite nanoplates grown at acidic to neutral pH. Nanoscale, 2021, 13, 17373-17385.	2.8	5
29	The controlling role of atmosphere in dawsonite versus gibbsite precipitation from tetrahedral aluminate species. Dalton Transactions, 2021, 50, 13438-13446.	1.6	1
30	Molecular Examination of Ion-Pair Competition in Alkaline Aluminate Solutions Using In Situ Liquid SIMS. Analytical Chemistry, 2021, 93, 1068-1075.	3.2	6
31	Theory-Guided Inelastic Neutron Scattering of Crystalline Alkaline Aluminate Salts Bearing Principal Motifs of Solution-State Species. Inorganic Chemistry, 2021, 60, 16223-16232.	1.9	4
32	No Hydrogen Bonding between Water and Hydrophilic Single Crystal MgO Surfaces?. Journal of Physical Chemistry C, 2021, 125, 26132-26138.	1.5	8
33	Analysis of the Fe 2p XPS for hematite Î± Fe2O3: Consequences of covalent bonding and orbital splittings on multiplet splittings. Journal of Chemical Physics, 2020, 152, 014704.	1.2	59
34	Ionâ€“ion interactions enhance aluminum solubility in alkaline suspensions of nano-gibbsite (Î±-Al(OH)₃) with sodium nitrite/nitrate. Physical Chemistry Chemical Physics, 2020, 22, 4368-4378.	1.3	19
35	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.	1.6	72
36	Covalency in Fe2O3 and FeO: Consequences for XPS satellite intensity. Journal of Chemical Physics, 2020, 153, 194702.	1.2	22

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37	Mechanisms of Al³⁺ Dimerization in Alkaline Solutions. Inorganic Chemistry, 2020, 59, 18181-18189.	1.9	8
38	Influence of soluble oligomeric aluminum on precipitation in the Alâ€“KOHâ€“H2O system. Physical Chemistry Chemical Physics, 2020, 22, 24677-24685.	1.3	7
39	Rethinking the magnetic properties of lepidocrocite: A density functional theory and cluster expansion study. Journal of Applied Physics, 2020, 128, .	1.1	1
40	Radiation-Induced Interfacial Hydroxyl Transformation on Boehmite and Gibbsite Basal Surfaces. Journal of Physical Chemistry C, 2020, 124, 22185-22191.	1.5	8
41	Nanoscale observations of Fe(<scp>ii</scp>)-induced ferrihydrite transformation. Environmental Science: Nano, 2020, 7, 2953-2967.	2.2	21
42	Citrate Controls Fe(II)-Catalyzed Transformation of Ferrihydrite by Complexation of the Labile Fe(III) Intermediate. Environmental Science & Technology, 2020, 54, 7309-7319.	4.6	56
43	Solid-State Recrystallization Pathways of Sodium Aluminate Hydroxy Hydrates. Inorganic Chemistry, 2020, 59, 6857-6865.	1.9	11
44	Vacancy ordering during selective oxidation of Î²-NiAl. Materialia, 2020, 12, 100783.	1.3	6
45	Two-step route to size and shape controlled gibbsite nanoplates and the crystal growth mechanism. CrystEngComm, 2020, 22, 2555-2565.	1.3	10
46	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.	1.5	0
47	Emerging investigator series: ion diffusivities in nanoconfined interfacial water films contribute to mineral carbonation thresholds. Environmental Science: Nano, 2020, 7, 1068-1081.	2.2	19
48	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.	2.2	21
49	Polaronic structure of excess electrons and holes for a series of bulk iron oxides. Physical Chemistry Chemical Physics, 2020, 22, 10699-10709.	1.3	13
50	Surface Hydration and Hydroxyl Configurations of Gibbsite and Boehmite Nanoplates. Journal of Physical Chemistry C, 2020, 124, 5275-5285.	1.5	21
51	Phase Transition and Liquid-like Superionic Conduction in Ag₂S. Journal of Physical Chemistry C, 2020, 124, 10150-10158.	1.5	9
52	Connecting particle interactions to agglomerate morphology and rheology of boehmite nanocrystal suspensions. Journal of Colloid and Interface Science, 2020, 572, 328-339.	5.0	16
53	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.	5.0	18
54	Evolution of Radicals from the Photolysis of High Ionic Strength Alkaline Nitrite Solutions. Journal of Physical Chemistry A, 2020, 124, 3019-3025.	1.1	4

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55	Effect of Cr(III) Adsorption on the Dissolution of Boehmite Nanoparticles in Caustic Solution. Environmental Science & Technology, 2020, 54, 6375-6384.	4.6	8
56	Intermediate Species in the Crystallization of Sodium Aluminate Hydroxy Hydrates. Journal of Physical Chemistry C, 2020, 124, 12337-12345.	1.5	10
57	Inference of principal species in caustic aluminate solutions through solid-state spectroscopic characterization. Dalton Transactions, 2020, 49, 5869-5880.	1.6	10
58	Electron transfer calculations between edge sharing octahedra in hematite, goethite, and annite. Geochimica Et Cosmochimica Acta, 2020, 291, 79-91.	1.6	15
59	The role of surface hydroxyls on the radiolysis of gibbsite and boehmite nanoplatelets. Journal of Hazardous Materials, 2020, 398, 122853.	6.5	18
60	A Filon-like integration strategy for calculating exact exchange in periodic boundary conditions: a plane-wave DFT implementation. Materials Theory, 2020, 4, .	2.2	5
61	Facet-Specific Photocatalytic Degradation of Organics by Heterogeneous Fenton Chemistry on Hematite Nanoparticles. Environmental Science & Technology, 2019, 53, 10197-10207.	4.6	101
62	Electron- and Thermal-Stimulated Synthesis of Water on Boehmite (Î³-AlOOH) Nanoplates. Journal of Physical Chemistry C, 2019, 123, 18986-18992.	1.5	8
63	Quantitative Review of Olivine Carbonation Kinetics: Reactivity Trends, Mechanistic Insights, and Research Frontiers. Environmental Science and Technology Letters, 2019, 6, 431-442.	3.9	31
64	Effect of structure and composition on the electronic excitation induced amorphization of La2Ti2â^'xZrxO7 ceramics. Scientific Reports, 2019, 9, 8190.	1.6	11
65	Facet-selective adsorption of Fe(<scp>ii</scp>) on hematite visualized by nanoscale secondary ion mass spectrometry. Environmental Science: Nano, 2019, 6, 2429-2440.	2.2	10
66	Reply to â€œComment on â€˜Roles of Hydration and Magnetism on the Structure of Ferrihydrite from First Principlesâ€™â€• ACS Earth and Space Chemistry, 2019, 3, 1581-1583.	1.2	4
67	Structure, Magnetism, and the Interaction of Water with Ti-Doped Fe3O4 Surfaces. Langmuir, 2019, 35, 13872-13879.	1.6	6
68	A Closer Look at Fe(II) Passivation of Goethite. ACS Earth and Space Chemistry, 2019, 3, 2717-2725.	1.2	22
69	Temperature Dependence of Self-Diffusion in Cr₂O₃ from First Principles. Journal of Physical Chemistry C, 2019, 123, 22139-22150.	1.5	12
70	Transformation of Gibbsite to Boehmite in Caustic Aqueous Solution at Hydrothermal Conditions. Crystal Growth and Design, 2019, 19, 5557-5567.	1.4	19
71	Cr(III) Adsorption by Cluster Formation on Boehmite Nanoplates in Highly Alkaline Solution. Environmental Science & Technology, 2019, 53, 11043-11055.	4.6	42
72	Cluster embedding of ionic systems: Point charges and extended ions. Journal of Chemical Physics, 2019, 151, 044107.	1.2	15

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73	Unraveling Gibbsite Transformation Pathways into LiAl-LDH in Concentrated Lithium Hydroxide. Inorganic Chemistry, 2019, 58, 12385-12394.	1.9	29
74	Redistribution of Electron Equivalents between Magnetite and Aqueous Fe2+ Induced by a Model Quinone Compound AQDS. Environmental Science & Technology, 2019, 53, 1863-1873.	4.6	18
75	Lateral water structure connects metal oxide nanoparticle faces. Journal of Materials Research, 2019, 34, 456-464.	1.2	4
76	Anomalously low activation energy of nanoconfined MgCO₃ precipitation. Chemical Communications, 2019, 55, 6835-6837.	2.2	25
77	Surface-Catalyzed Oxygen Exchange during Mineral Carbonation in Nanoscale Water Films. Journal of Physical Chemistry C, 2019, 123, 12871-12885.	1.5	21
78	Natural, incidental, and engineered nanomaterials and their impacts on the Earth system. Science, 2019, 363, .	6.0	479
79	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.	3.3	52
80	Iron Redox Chemistry and Its Environmental Impact: A Virtual Special Issue. ACS Earth and Space Chemistry, 2019, 3, 2374-2375.	1.2	5
81	Synthesis of 2D Hexagonal Hematite Nanosheets and the Crystal Growth Mechanism. Inorganic Chemistry, 2019, 58, 16727-16735.	1.9	32
82	Reductive Dissolution Mechanisms at the Hematite-Electrolyte Interface Probed by in Situ X-ray Scattering. Journal of Physical Chemistry C, 2019, 123, 8077-8085.	1.5	8
83	Energetics and the Role of Defects in Fe(II)-Catalyzed Goethite Recrystallization from Molecular Simulations. ACS Earth and Space Chemistry, 2019, 3, 262-272.	1.2	18
84	Radiocesium interaction with clay minerals: Theory and simulation advances Postâ€“Fukushima. Journal of Environmental Radioactivity, 2019, 210, 105809.	0.9	7
85	Roles of Hydration and Magnetism on the Structure of Ferrihydrite from First Principles. ACS Earth and Space Chemistry, 2019, 3, 70-78.	1.2	23
86	Radiocesium interaction with clay minerals: Theory and simulation advances Postâ€“Fukushima. Journal of Environmental Radioactivity, 2018, 189, 135-145.	0.9	60
87	Surface Charge Effects on Fe(II) Sorption and Oxidation at (110) Goethite Surfaces. Journal of Physical Chemistry C, 2018, 122, 10059-10066.	1.5	10
88	Radiolytic stability of gibbsite and boehmite with adsorbed water. Journal of Nuclear Materials, 2018, 501, 224-233.	1.3	30
89	Electrochemical Interfaces: Potentialâ€Specific Structure at the Hematiteâ€“Electrolyte Interface (Adv.) Tj ETQq1 1 0.784314 rgBT /O	7.8	1
90	Resolving Iron(II) Sorption and Oxidative Growth on Hematite (001) Using Atom Probe Tomography. Journal of Physical Chemistry C, 2018, 122, 3903-3914.	1.5	26

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91	Synthesis of nanometer-sized fayalite and magnesium-iron(II) mixture olivines. Journal of Colloid and Interface Science, 2018, 515, 129-138.	5.0	19
92	The Role of Defects in Fe(II)â€“Goethite Electron Transfer. Environmental Science & Technology, 2018, 52, 2751-2759.	4.6	76
93	Consequences of realistic embedding for the L_{2,3} edge XAS of Î±-Fe₂O₃. Physical Chemistry Chemical Physics, 2018, 20, 4396-4403.	1.3	13
94	Size and Morphology Controlled Synthesis of Boehmite Nanoplates and Crystal Growth Mechanisms. Crystal Growth and Design, 2018, 18, 3596-3606.	1.4	82
95	Free-Energy Landscape of the Dissolution of Gibbsite at High pH. Journal of Physical Chemistry Letters, 2018, 9, 1809-1814.	2.1	25
96	Potentialâ€Specific Structure at the Hematiteâ€“Electrolyte Interface. Advanced Functional Materials, 2018, 28, 1705618.	7.8	16
97	²⁷Al Pulsed Field Gradient, Diffusionâ€“NMR Spectroscopy of Solvation Dynamics and Ion Pairing in Alkaline Aluminate Solutions. Journal of Physical Chemistry B, 2018, 122, 10907-10912.	1.2	15
98	Boehmite and Gibbsite Nanoplates for the Synthesis of Advanced Alumina Products. ACS Applied Nano Materials, 2018, 1, 7115-7128.	2.4	79
99	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.	1.6	25
100	Acidity Constants of the Hematiteâ€“Liquid Water Interface from Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 5574-5582.	2.1	25
101	Impact of Solution Chemistry and Particle Anisotropy on the Collective Dynamics of Oriented Aggregation. ACS Nano, 2018, 12, 10114-10122.	7.3	40
102	X-ray Linear Dichroism in Apatite. Journal of the American Chemical Society, 2018, 140, 11698-11704.	6.6	19
103	Accessing crystalâ€“crystal interaction forces with oriented nanocrystal atomic force microscopy probes. Nature Protocols, 2018, 13, 2005-2030.	5.5	12
104	Surface Chemistry Affects the Efficacy of the Hydration Force between Two ZnO(101Ì…0) Surfaces. Journal of Physical Chemistry C, 2018, 122, 12259-12266.	1.5	16
105	First-Principles Investigation of Native Interstitial Diffusion in Cr₂O₃. Journal of Physical Chemistry C, 2018, 122, 12984-12993.	1.5	19
106	A Thermodynamic Model for ZrO2(am) Solubility at 25ÂÂ°C in the Ca2+â€“Na+â€“H+â€“Clâ^'â€“OHâ^'â€“H2O System: A Critical Review. Journal of Solution Chemistry, 2018, 47, 855-891.	0.6	11
107	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.	2.3	15
108	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.	1.2	34

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109	Iron Dissolution from Goethite (Î±-FeOOH) Surfaces in Water by Ab Initio Enhanced Free-Energy Simulations. Journal of Physical Chemistry C, 2018, 122, 16086-16091.	1.5	33
110	In Situ ²⁷Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions above and below Saturation with Respect to Gibbsite. Inorganic Chemistry, 2018, 57, 11864-11873.	1.9	33
111	Facet-dependent contaminant removal properties of hematite nanocrystals and their environmental implications. Environmental Science: Nano, 2018, 5, 1790-1806.	2.2	93
112	Technetium Stabilization in Low-Solubility Sulfide Phases: A Review. ACS Earth and Space Chemistry, 2018, 2, 532-547.	1.2	36
113	Water Structure Controls Carbonic Acid Formation in Adsorbed Water Films. Journal of Physical Chemistry Letters, 2018, 9, 4988-4994.	2.1	16
114	Reversible Fe(<scp>ii</scp>) uptake/release by magnetite nanoparticles. Environmental Science: Nano, 2018, 5, 1545-1555.	2.2	20
115	Vacancies and Vacancy-Mediated Self Diffusion in Cr₂O₃: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 1817-1831.	1.5	24
116	Dynamic Stabilization of Metal Oxideâ€“Water Interfaces. Journal of the American Chemical Society, 2017, 139, 2581-2584.	6.6	60
117	Direction-specific van der Waals attraction between rutile TiO ₂ nanocrystals. Science, 2017, 356, 434-437.	6.0	103
118	Electron Mobility and Trapping in Ferrihydrite Nanoparticles. ACS Earth and Space Chemistry, 2017, 1, 216-226.	1.2	21
119	Stochastic Simulation of Isotopic Exchange Mechanisms for Fe(II)-Catalyzed Recrystallization of Goethite. Environmental Science & Technology, 2017, 51, 7552-7559.	4.6	20
120	Improving the Performance of Hybrid Functional-Based Molecular Dynamics Simulation through Screening of Hartreeâ€“Fock Exchange Forces. Journal of Chemical Theory and Computation, 2017, 13, 2178-2184.	2.3	9
121	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.	1.5	14
122	Water Solubility at Saturation for CO₂â€“CH₄ Mixtures at 323.2 K and 9.000 MPa. Journal of Chemical & Engineering Data, 2017, 62, 1608-1614.	1.0	25
123	Direction-specific interaction forces underlying zinc oxide crystal growth by oriented attachment. Nature Communications, 2017, 8, 835.	5.8	80
124	Tipping Point for Expansion of Layered Aluminosilicates in Weakly Polar Solvents: Supercritical CO₂. ACS Applied Materials & Interfaces, 2017, 9, 36783-36791.	4.0	38
125	Transmutation effects on long-term Cs retention in phyllosilicate minerals from first principles. Physical Chemistry Chemical Physics, 2017, 19, 27007-27014.	1.3	4
126	Impact of Ti Incorporation on Hydroxylation and Wetting of Fe₃O₄. Journal of Physical Chemistry C, 2017, 121, 19288-19295.	1.5	10

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127	First-Principles Fe L_{2,3}-Edge and O K-Edge XANES and XMCD Spectra for Iron Oxides. Journal of Physical Chemistry A, 2017, 121, 7613-7618.	1.1	30
128	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.	1.1	22
129	Electron Transfer Pathways Facilitating U(VI) Reduction by Fe(II) on Al- vs Fe-Oxides. Journal of Physical Chemistry C, 2017, 121, 19887-19903.	1.5	17
130	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.	1.5	41
131	A thermodynamic model for the solubility of HfO₂(am) in the aqueous K^{â€‰+}â€‰â€“â€‰HCO₃ <sup>â€‰â€“â€‰CO₃ ^{2â€‰â€“}â€‰OH^{â€‰â€“}â€‰â€“â€‰H₂O system. Radiochimica Acta, 2017, 105, 637-647.	1.5	6
132	Fast Synthesis of Gibbsite Nanoplates and Process Optimization using Box-Behnken Experimental Design. Crystal Growth and Design, 2017, 17, 6801-6808.	1.4	47
133	Redox potentials in the decaheme cytochrome MtrF: Poissonâ€“Boltzmann vs. molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10028.	3.3	3
134	Tc(VII) and Cr(VI) Interaction with Naturally Reduced Ferruginous Smectite from a Redox Transition Zone. Environmental Science & Technology, 2017, 51, 9042-9052.	4.6	38
135	Trends in micaâ€“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.	3.3	56
136	Probing size-dependent electrokinetics of hematite aggregates. Journal of Colloid and Interface Science, 2017, 488, 218-224.	5.0	12
137	Analysis of X-ray adsorption edges: L2,3 edge of FeCl4â^. Journal of Chemical Physics, 2017, 147, 224306.	1.2	16
138	Origin of 6-fold coordinated aluminum at (010)-type pyrophyllite edges. AIP Advances, 2017, 7, 055211.	0.6	6
139	Reply to "Comments 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.	0.6	2
140	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.	0.6	6
141	Molecular Simulation of Cesium Adsorption at the Basal Surface of Phyllosilicate Minerals. Clays and Clay Minerals, 2016, 64, 389-400.	0.6	30
142	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.	1.6	27
143	Hematite(001)-liquid water interface from hybrid density functional-based molecular dynamics. Journal of Physics Condensed Matter, 2016, 28, 394001.	0.7	20
144	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.	1.6	38

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145	The origin of facet selectivity and alignment in anatase TiO₂nanoparticles in electrolyte solutions: implications for oriented attachment in metal oxides. Nanoscale, 2016, 8, 19714-19725.	2.8	45
146	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.	3.0	14
147	In Situ Natural Abundance ¹⁷O and ²⁵Mg NMR Investigation of Aqueous Mg(OH)₂ Dissolution in the Presence of Supercritical CO₂. Environmental Science & Technology, 2016, 50, 12373-12384.	4.6	7
148	Size dependent microbial oxidation and reduction of magnetite nano- and micro-particles. Scientific Reports, 2016, 6, 30969.	1.6	34
149	Issues concerning the determination of solubility products of sparingly soluble crystalline solids: solubility of HfO₂(cr). Radiochimica Acta, 2016, 104, 583-592.	0.5	5
150	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.	0.9	11
151	Fast Interconversion of Hydrogen Bonding at the Hematite (001)â€“Liquid Water Interface. Journal of Physical Chemistry Letters, 2016, 7, 1155-1160.	2.1	42
152	Capturing ultrafast photoinduced local structural distortions of BiFeO3. Scientific Reports, 2015, 5, 15098.	1.6	21
153	Flavin Binding to the Deca-heme Cytochrome MtrC: Insights from Computational Molecular Simulation. Biophysical Journal, 2015, 109, 2614-2624.	0.2	16
154	Characterizing mineralogy and redox reactivity in potential host rocks for a UK geological disposal facility. Mineralogical Magazine, 2015, 79, 1353-1367.	0.6	6
155	Heterogeneous growth of cadmium and cobalt carbonate phases at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mfenced open="(" close=")"><mml:mrow><mml:mn>10</mml:mn><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo stretchy="true">Â¯</mml:mo></mml:mover><mml:mn>4</mml:mn></mml:mrow></mml:mfenced></mml:math> calcite surface. Chemical Geology, 2015, 397, 24-36.	1.4	18
156	Charge Transport at Ti-Doped Hematite (001)/Aqueous Interfaces. Chemistry of Materials, 2015, 27, 1665-1673.	3.2	26
157	Atom Exchange between Aqueous Fe(II) and Structural Fe in Clay Minerals. Environmental Science & Technology, 2015, 49, 2786-2795.	4.6	46
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