# Kevin M Rosso

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Electrically conductive bacterial nanowires produced by Shewanella oneidensis strain MR-1 and other microorganisms. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 11358-11363. | 3.3 | 1,629 |
| 2 | Nanostructures and lithium electrochemical reactivity of lithium titanites and titanium oxides: A review. Journal of Power Sources, 2009, 192, 588-598. | 4.0 | 804 |
| 3 | Natural, incidental, and engineered nanomaterials and their impacts on the Earth system. Science, 2019, 363, . | 6.0 | 479 |
| 4 | Role of extracellular polymeric substances in bioflocculation of activated sludge microorganisms under glucose-controlled conditions. Water Research, 2010, 44, 4505-4516. | 5.3 | 396 |
| 5 | Linked Reactivity at Mineral-Water Interfaces Through Bulk Crystal Conduction. Science, 2008, 320, 218-222. | 6.0 | 327 |
| 6 | The roles of outer membrane cytochromes of <i>Shewanella</i> and <i>Geobacter</i> in extracellular electron transfer. Environmental Microbiology Reports, 2009, 1, 220-227. | 1.0 | 285 |
| 7 | Charge transport in metal oxides: A theoretical study of hematite Î±-Fe2O3. Journal of Chemical Physics, 2005, 122, 144305. | 1.2 | 281 |
| 8 | An ab initio model of electron transport in hematite (Î±-Fe2O3) basal planes. Journal of Chemical Physics, 2003, 118, 6455-6466. | 1.2 | 274 |
| 9 | Fe(II) Redox Chemistry in the Environment. Chemical Reviews, 2021, 121, 8161-8233. | 23.0 | 242 |
| 10 | Redox cycling of Fe(II) and Fe(III) in magnetite by Fe-metabolizing bacteria. Science, 2015, 347, 1473-1476. | 6.0 | 239 |
| 11 | Multi-haem cytochromes in<i>Shewanella oneidensis</i>MR-1: structures, functions and opportunities. Journal of the Royal Society Interface, 2015, 12, 20141117. | 1.5 | 193 |
| 12 | Identification and Characterization of MtoA: A Decaheme c-Type Cytochrome of the Neutrophilic Fe(II)-Oxidizing Bacterium Sideroxydans lithotrophicus ES-1. Frontiers in Microbiology, 2012, 3, 37. | 1.5 | 186 |
| 13 | Molecular Underpinnings of Fe(III) Oxide Reduction by Shewanella Oneidensis MR-1. Frontiers in Microbiology, 2012, 3, 50. | 1.5 | 186 |
| 14 | A transâ€outer membrane porinâ€cytochrome protein complex for extracellular electron transfer by <scp><i>G</i></scp><i>eobacter sulfurreducens</i>â€…<scp>PCA</scp>. Environmental Microbiology Reports, 2014, 6, 776-785. | 1.0 | 178 |
| 15 | Electron flow in multiheme bacterial cytochromes is a balancing act between heme electronic interaction and redox potentials. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 611-616. | 3.3 | 171 |
| 16 | Electron Small Polarons and Their Mobility in Iron (Oxyhydr)oxide Nanoparticles. Science, 2012, 337, 1200-1203. | 6.0 | 166 |
| 17 | Fe(II)-Catalyzed Recrystallization of Goethite Revisited. Environmental Science & Technology, 2014, 48, 11302-11311. | 4.6 | 160 |
| 18 | In Situ Infrared Spectroscopic Study of Forsterite Carbonation in Wet Supercritical CO<sub>2</sub>. Environmental Science & Technology, 2011, 45, 6204-6210. | 4.6 | 153 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Mtr extracellular electron-transfer pathways in Fe(III)-reducing or Fe(II)-oxidizing bacteria: a genomic perspective. Biochemical Society Transactions, 2012, 40, 1261-1267. | 1.6 | 150 |
| 20 | The interaction of pyrite {100} surfaces with O<sub>2</sub>and H<sub>2</sub>O; fundamental oxidation mechanisms. American Mineralogist, 1999, 84, 1549-1561. | 0.9 | 137 |
| 21 | <I>Ab initio</I> determination of edge surface structures for dioctahedral 2:1 phyllosilicates: implications for acid-base for reactivity. Clays and Clay Minerals, 2003, 51, 359-371. | 0.6 | 135 |
| 22 | Reversible ketone hydrogenation and dehydrogenation for aqueous organic redox flow batteries. Science, 2021, 372, 836-840. | 6.0 | 135 |
| 23 | The structure of hematite (Î±-Fe2O3) (001) surfaces in aqueous media: scanning tunneling microscopy and resonant tunneling calculations of coexisting O and Fe terminations. Geochimica Et Cosmochimica Acta, 2003, 67, 985-1000. | 1.6 | 125 |
| 24 | The proximity effect on semiconducting mineral surfaces: a new aspect of mineral surface reactivity and surface complexation theory?. Geochimica Et Cosmochimica Acta, 2001, 65, 2641-2649. | 1.6 | 123 |
| 25 | Atomically resolved electronic structure of pyrite {100} surfaces; an experimental and theoretical investigation with implications for reactivity. American Mineralogist, 1999, 84, 1535-1548. | 0.9 | 118 |
| 26 | Bond-valence methods for pKa prediction: critical reanalysis and a new approach. Geochimica Et Cosmochimica Acta, 2004, 68, 2025-2042. | 1.6 | 118 |
| 27 | <i>In Situ</i> Molecular Spectroscopic Evidence for CO<sub>2</sub> Intercalation into Montmorillonite in Supercritical Carbon Dioxide. Langmuir, 2012, 28, 7125-7128. | 1.6 | 117 |
| 28 | Spectroscopic Characterization of Extracellular Polymeric Substances from <i>Escherichia coli</i> and <i>Serratia marcescens</i>: Suppression Using Sub-Inhibitory Concentrations of Bismuth Thiols. Biomacromolecules, 2008, 9, 3079-3089. | 2.6 | 113 |
| 29 | Influence of Dynamical Conditions on the Reduction of U<sup>VI</sup> at the Magnetiteâ<sup>~</sup>Solution Interface. Environmental Science & Technology, 2010, 44, 170-176. | 4.6 | 110 |
| 30 | Connecting Observations of Hematite (Î±-Fe<sub>2</sub>O<sub>3</sub>) Growth Catalyzed by Fe(II). Environmental Science & Technology, 2010, 44, 61-67. | 4.6 | 110 |
| 31 | Combined <sup>6,7</sup>Li NMR and Molecular Dynamics Study of Li Diffusion in Li<sub>2</sub>TiO<sub>3</sub>. Journal of Physical Chemistry C, 2009, 113, 20108-20116. | 1.5 | 107 |
| 32 | The role of H2O in the carbonation of forsterite in supercritical CO2. International Journal of Greenhouse Gas Control, 2011, 5, 1081-1092. | 2.3 | 103 |
| 33 | Direction-specific van der Waals attraction between rutile TiO <sub>2</sub> nanocrystals. Science, 2017, 356, 434-437. | 6.0 | 103 |
| 34 | Nonlocal bacterial electron transfer to hematite surfaces. Geochimica Et Cosmochimica Acta, 2003, 67, 1081-1087. | 1.6 | 102 |
| 35 | Facet-Specific Photocatalytic Degradation of Organics by Heterogeneous Fenton Chemistry on Hematite Nanoparticles. Environmental Science & Technology, 2019, 53, 10197-10207. | 4.6 | 101 |
| 36 | Iron Atom Exchange between Hematite and Aqueous Fe(II). Environmental Science & Technology, 2015, 49, 8479-8486. | 4.6 | 99 |

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| 37 | Self-similar mesocrystals form via interface-driven nucleation and assembly. Nature, 2021, 590, 416-422. | 13.7 | 98 |
| 38 | Reaction of water-saturated supercritical CO2 with forsterite: Evidence for magnesite formation at low temperatures. Geochimica Et Cosmochimica Acta, 2012, 91, 271-282. | 1.6 | 97 |
| 39 | <i>In Situ</i> Study of CO<sub>2</sub> and H<sub>2</sub>O Partitioning between Naâ€“Montmorillonite and Variably Wet Supercritical Carbon Dioxide. Langmuir, 2014, 30, 6120-6128. | 1.6 | 97 |
| 40 | CO<sub>2</sub> Sorption to Subsingle Hydration Layer Montmorillonite Clay Studied by Excess Sorption and Neutron Diffraction Measurements. Environmental Science & Technology, 2013, 47, 205-211. | 4.6 | 96 |
| 41 | Facet-dependent contaminant removal properties of hematite nanocrystals and their environmental implications. Environmental Science: Nano, 2018, 5, 1790-1806. | 2.2 | 93 |
| 42 | Kinetics of Reduction of Fe(III) Complexes by Outer Membrane Cytochromes MtrC and OmcA of<i>Shewanella oneidensis</i>MR-1. Applied and Environmental Microbiology, 2008, 74, 6746-6755. | 1.4 | 89 |
| 43 | 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. Journal of Physical Chemistry C, 2010, 114, 4126-4134. | 1.5 | 89 |
| 44 | In Situ X-ray Diffraction Study of Na<sup>+</sup> Saturated Montmorillonite Exposed to Variably Wet Super Critical CO<sub>2</sub>. Environmental Science & Technology, 2012, 46, 4241-4248. | 4.6 | 89 |
| 45 | U(VI) Sorption and Reduction Kinetics on the Magnetite (111) Surface. Environmental Science & Technology, 2012, 46, 3821-3830. | 4.6 | 84 |
| 46 | Size and Morphology Controlled Synthesis of Boehmite Nanoplates and Crystal Growth Mechanisms. Crystal Growth and Design, 2018, 18, 3596-3606. | 1.4 | 82 |
| 47 | Computer simulation of electron transfer at hematite surfaces. Geochimica Et Cosmochimica Acta, 2006, 70, 1888-1903. | 1.6 | 80 |
| 48 | Synthesis and properties of titanomagnetite (Fe3âˆ’xTixO4) nanoparticles: A tunable solid-state Fe(II/III) redox system. Journal of Colloid and Interface Science, 2012, 387, 24-38. | 5.0 | 80 |
| 49 | Direction-specific interaction forces underlying zinc oxide crystal growth by oriented attachment. Nature Communications, 2017, 8, 835. | 5.8 | 80 |
| 50 | Surface potentials of (001), (012), (113) hematite (Î±-Fe2O3) crystal faces in aqueous solution. Physical Chemistry Chemical Physics, 2013, 15, 13911. | 1.3 | 79 |
| 51 | in Situ High-Pressure X-ray Diffraction Study. Environmental Science & Technology, 2013, 47, 174-181. | 4.6 | 79 |
| 52 | Boehmite and Gibbsite Nanoplates for the Synthesis of Advanced Alumina Products. ACS Applied Nano Materials, 2018, 1, 7115-7128. | 2.4 | 79 |
| 53 | Thermodynamics of Electron Flow in the Bacterial Deca-heme Cytochrome MtrF. Journal of the American Chemical Society, 2012, 134, 9868-9871. | 6.6 | 78 |
| 54 | 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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| 55 | Surface structure effects on direct reduction of iron oxides by Shewanella oneidensis. Geochimica Et Cosmochimica Acta, 2003, 67, 4489-4503. | 1.6 | 76 |
| 56 | Structure and oxidation state of hematite surfaces reacted with aqueous Fe(II) at acidic and neutral pH. Geochimica Et Cosmochimica Acta, 2010, 74, 1498-1512. | 1.6 | 76 |
| 57 | The Role of Defects in Fe(II)â€"Goethite Electron Transfer. Environmental Science & Technology, 2018, 52, 2751-2759. | 4.6 | 76 |
| 58 | Mechanism of Li<sup>+</sup>/Electron Conductivity in Rutile and Anatase TiO<sub>2</sub> Nanoparticles. Journal of Physical Chemistry C, 2010, 114, 20277-20283. | 1.5 | 73 |
| 59 | Outer-sphere electron transfer kinetics of metal ion oxidation by molecular oxygen. Geochimica Et Cosmochimica Acta, 2002, 66, 4223-4233. | 1.6 | 72 |
| 60 | 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 |
| 61 | Oxygen Vacancies and Ordering of dâ€levels Control Voltage Suppression in Oxide Cathodes: the Case of Spinel LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4â€<i>Î´</i></sub>. Advanced Functional Materials, 2013, 23, 5530-5535. | 7.8 | 69 |
| 62 | Ab Initio Calculation of Homogeneous Outer Sphere Electron Transfer Rates:Â Application to M(OH2)63+/2+Redox Couples. Journal of Physical Chemistry A, 2000, 104, 6718-6725. | 1.1 | 67 |
| 63 | Facet-Dependent Photodegradation of Methylene Blue by Hematite Nanoplates in Visible Light. Environmental Science & Technology, 2021, 55, 677-688. | 4.6 | 67 |
| 64 | Bond-valence methods for pKa prediction. II. Bond-valence, electrostatic, molecular geometry, and solvation effects. Geochimica Et Cosmochimica Acta, 2006, 70, 4057-4071. | 1.6 | 66 |
| 65 | Reactivity of Sulfide Mineral Surfaces. Reviews in Mineralogy and Geochemistry, 2006, 61, 557-607. | 2.2 | 65 |
| 66 | Structure, charge distribution, and electron hopping dynamics in magnetite (Fe3O4) (100) surfaces from first principles. Geochimica Et Cosmochimica Acta, 2010, 74, 4234-4248. | 1.6 | 65 |
| 67 | Lithium diffusion in Li4Ti5O12 at high temperatures. Journal of Power Sources, 2011, 196, 2211-2220. | 4.0 | 65 |
| 68 | Electron density distribution and bond critical point properties for forsterite, Mg2 SiO4, determined with synchrotron single crystal X-ray diffraction data. Physics and Chemistry of Minerals, 2005, 32, 301-313. | 0.3 | 64 |
| 69 | Kinetic Monte Carlo model of charge transport in hematite (Î±-Fe2O3). Journal of Chemical Physics, 2007, 127, 124706. | 1.2 | 63 |
| 70 | Charge and Ion Transport in NiO and Aspects of Ni Oxidation from First Principles. Journal of Physical Chemistry C, 2012, 116, 1948-1954. | 1.5 | 62 |
| 71 | Molecular Dynamics Study of Fe(II) Adsorption, Electron Exchange, and Mobility at Goethite (Î±-FeOOH) Surfaces. Journal of Physical Chemistry C, 2015, 119, 3111-3123. | 1.5 | 62 |
| 72 | Molecular Dynamics Characterization of Rutile-Anatase Interfaces. Journal of Physical Chemistry C, 2007, 111, 9290-9298. | 1.5 | 61 |

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| 73 | Molecular Computational Investigation of Electron-Transfer Kinetics Across Cytochromeâ˜'Iron Oxide Interfaces. Journal of Physical Chemistry C, 2007, 111, 11363-11375. | 1.5 | 61 |
| 74 | In Situ Infrared Spectroscopic Study of Brucite Carbonation in Dry to Water-Saturated Supercritical Carbon Dioxide. Journal of Physical Chemistry A, 2012, 116, 4768-4777. | 1.1 | 61 |
| 75 | Ab initio modeling of Fe(<scp>ii</scp>) adsorption and interfacial electron transfer at goethite (Ã®Â±-FeOOH) surfaces. Physical Chemistry Chemical Physics, 2015, 17, 14518-14531. | 1.3 | 60 |
| 76 | Dynamic Stabilization of Metal Oxideâ€"Water Interfaces. Journal of the American Chemical Society, 2017, 139, 2581-2584. | 6.6 | 60 |
| 77 | Radiocesium interaction with clay minerals: Theory and simulation advances Postâ€"Fukushima. Journal of Environmental Radioactivity, 2018, 189, 135-145. | 0.9 | 60 |
| 78 | Electron transfer in environmental systems: a frontier for theoretical chemistry. Theoretical Chemistry Accounts, 2006, 116, 124-136. | 0.5 | 59 |
| 79 | Effect of Chemical Lithium Insertion into Rutile TiO<sub>2</sub> Nanorods. Journal of Physical Chemistry C, 2009, 113, 14567-14574. | 1.5 | 59 |
| 80 | Identification of Simultaneous U(VI) Sorption Complexes and U(IV) Nanoprecipitates on the Magnetite (111) Surface. Environmental Science & Technology, 2012, 46, 3811-3820. | 4.6 | 59 |
| 81 | Analysis of the Fe 2p XPS for hematite Ã®Â± Fe2O3: Consequences of covalent bonding and orbital splittings on multiplet splittings. Journal of Chemical Physics, 2020, 152, 014704. | 1.2 | 59 |
| 82 | Metal oxidation kinetics and the transition from thin to thick films. Physical Chemistry Chemical Physics, 2012, 14, 14534. | 1.3 | 58 |
| 83 | Electron tunneling properties of outer-membrane decaheme cytochromes from Shewanella oneidensis. Geochimica Et Cosmochimica Acta, 2007, 71, 543-555. | 1.6 | 56 |
| 84 | Bismuth dimercaptopropanol (BisBAL) inhibits the expression of extracellular polysaccharides and proteins by <i>Brevundimonas diminuta</i>: Implications for membrane microfiltration. Biotechnology and Bioengineering, 2008, 99, 634-643. | 1.7 | 56 |
| 85 | 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 |
| 86 | 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 |
| 87 | 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. | 0.3 | 55 |
| 88 | Structure and Charge Hopping Dynamics in Green Rust. Journal of Physical Chemistry C, 2007, 111, 11414-11423. | 1.5 | 53 |
| 89 | A Shell Model for Atomistic Simulation of Charge Transfer in Titania. Journal of Physical Chemistry C, 2008, 112, 7678-7688. | 1.5 | 53 |
| 90 | Dynamics of Coupled Lithium/Electron Diffusion in TiO<sub>2</sub> Polymorphs. Journal of Physical Chemistry C, 2009, 113, 20998-21007. | 1.5 | 53 |

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| 91 | Insights into the Mechanism of Fe(II) Adsorption and Oxidation at Feâ€"Clay Mineral Surfaces from First-Principles Calculations. Journal of Physical Chemistry C, 2013, 117, 22880-22886. | 1.5 | 53 |
| 92 | 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 |
| 93 | Mechanisms of Electron Transfer in Two Decaheme Cytochromes from a Metal-Reducing Bacterium. Journal of Physical Chemistry B, 2007, 111, 12857-12864. | 1.2 | 51 |
| 94 | Simple kinetic Monte Carlo models for dissolution pitting induced by crystal defects. Journal of Chemical Physics, 2008, 129, 204106. | 1.2 | 50 |
| 95 | Technetium Incorporation into Hematite (Î±-Fe<sub>2</sub>O<sub>3</sub>). Environmental Science & Technology, 2010, 44, 5855-5861. | 4.6 | 48 |
| 96 | Electronic Coupling between Heme Electron-Transfer Centers and Its Decay with Distance Depends Strongly on Relative Orientation. Journal of Physical Chemistry B, 2006, 110, 15582-15588. | 1.2 | 47 |
| 97 | Evidence for Carbonate Surface Complexation during Forsterite Carbonation in Wet Supercritical Carbon Dioxide. Langmuir, 2015, 31, 7533-7543. | 1.6 | 47 |
| 98 | Fast Synthesis of Gibbsite Nanoplates and Process Optimization using Box-Behnken Experimental Design. Crystal Growth and Design, 2017, 17, 6801-6808. | 1.4 | 47 |
| 99 | Reorganization energy associated with small polaron mobility in iron oxide. Journal of Chemical Physics, 2004, 120, 7050-7054. | 1.2 | 46 |
| 100 | Self-Exchange Electron Transfer Kinetics and Reduction Potentials for Anthraquinone Disulfonate. Journal of Physical Chemistry A, 2004, 108, 3292-3303. | 1.1 | 46 |
| 101 | Atom Exchange between Aqueous Fe(II) and Structural Fe in Clay Minerals. Environmental Science & Technology, 2015, 49, 2786-2795. | 4.6 | 46 |
| 102 | Structures and energies of AlOOH and FeOOH polymorphs from plane wave pseudopotential calculations. American Mineralogist, 2001, 86, 312-317. | 0.9 | 45 |
| 103 | Thermodynamics of the magnetite-ulvospinel (Fe3O4-Fe2TiO4) solid solution. American Mineralogist, 2012, 97, 1330-1338. | 0.9 | 45 |
| 104 | The origin of facet selectivity and alignment in anatase TiO<sub>2</sub>nanoparticles in electrolyte solutions: implications for oriented attachment in metal oxides. Nanoscale, 2016, 8, 19714-19725. | 2.8 | 45 |
| 105 | Adatom Fe(III) on the hematite surface: Observation of a key reactive surface species. Geochemical Transactions, 2004, 5, 1. | 1.8 | 44 |
| 106 | Chromium(III) Hydroxide Solubility in the Aqueous K+-H+-OHâˆ'-CO2-HCO 3 âˆ' -CO 3 2âˆ' -H2O System: AÂThermodynamic Model. Journal of Solution Chemistry, 2007, 36, 1261-1285. | 0.6 | 43 |
| 107 | Shared and Closed-Shell Oâˆ'O Interactions in Silicates. Journal of Physical Chemistry A, 2008, 112, 3693-3699. | 1.1 | 43 |
| 108 | Computer simulation of the light yield nonlinearity of inorganic scintillators. Journal of Applied Physics, 2009, 105, . | 1.1 | 43 |

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|---|---|---|---|
| 109 | Fe<sub>3â€“<i>x</i></sub>Ti<sub><i>x</i></sub>O<sub>4</sub> Nanoparticles as Tunable Probes of Microbial Metal Oxidation. Journal of the American Chemical Society, 2013, 135, 8896-8907. | 6.6 | 43 |
| 110 | Electron Exchange and Conduction in Nontronite from First-Principles. Journal of Physical Chemistry C, 2013, 117, 2032-2040. | 1.5 | 43 |
| 111 | Comparative reactivity study of forsterite and antigorite in wet supercritical CO2 by in situ infrared spectroscopy. International Journal of Greenhouse Gas Control, 2013, 18, 246-255. | 2.3 | 43 |
| 112 | Electron transport in pure and substituted iron oxyhydroxides by small-polaron migration. Journal of Chemical Physics, 2014, 140, 234701. | 1.2 | 43 |
| 113 | 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 |
| 114 | Cr(III) Adsorption by Cluster Formation on Boehmite Nanoplates in Highly Alkaline Solution. Environmental Science & Technology, 2019, 53, 11043-11055. | 4.6 | 42 |
| 115 | Charge transfer in FeO: A combined molecular-dynamics and ab initio study. Journal of Chemical Physics, 2005, 123, 224712. | 1.2 | 41 |
| 116 | Electron Density Distributions Calculated for the Nickel Sulfides Millerite, Vaesite, and Heazlewoodite and Nickel Metal:Â A Case for the Importance of Niâ˜'Ni Bond Paths for Electron Transport. Journal of Physical Chemistry B, 2005, 109, 21788-21795. | 1.2 | 41 |
| 117 | Transitions in Al Coordination during Gibbsite Crystallization Using High-Field <sup>27</sup>Al and <sup>23</sup>Na MAS NMR Spectroscopy. Journal of Physical Chemistry C, 2017, 121, 27555-27562. | 1.5 | 41 |
| 118 | Impact of Solution Chemistry and Particle Anisotropy on the Collective Dynamics of Oriented Aggregation. ACS Nano, 2018, 12, 10114-10122. | 7.3 | 40 |
| 119 | Proximity effects on semiconducting mineral surfaces II:. Geochimica Et Cosmochimica Acta, 2003, 67, 941-953. | 1.6 | 39 |
| 120 | Charge transport in micas: The kinetics of FeII/III electron transfer in the octahedral sheet. Journal of Chemical Physics, 2003, 119, 9207-9218. | 1.2 | 39 |
| 121 | Clay Hydration/dehydration in Dry to Water-saturated Supercritical CO2: Implications for Caprock Integrity. Energy Procedia, 2013, 37, 5443-5448. | 1.8 | 39 |
| 122 | Cell adhesion of Shewanella oneidensisto iron oxide minerals: Effect of different single crystal faces. Geochemical Transactions, 2005, 6, 1. | 1.8 | 38 |
| 123 | Heterogeneous Reduction of PuO<sub>2</sub> with Fe(II): Importance of the Fe(III) Reaction Product. Environmental Science & Technology, 2011, 45, 3952-3958. | 4.6 | 38 |
| 124 | Kinetic Monte Carlo Study of Ambipolar Lithium Ion and Electronâ€“Polaron Diffusion into Nanostructured TiO<sub>2</sub>. Journal of Physical Chemistry Letters, 2012, 3, 2076-2081. | 2.1 | 38 |
| 125 | The Effect of pH and Time on the Extractability and Speciation of Uranium(VI) Sorbed to SiO<sub>2</sub>. Environmental Science & Technology, 2012, 46, 6604-6611. | 4.6 | 38 |
| 126 | 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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| 127 | Tipping Point for Expansion of Layered Aluminosilicates in Weakly Polar Solvents: Supercritical CO<sub>2</sub>. ACS Applied Materials & Interfaces, 2017, 9, 36783-36791. | 4.0 | 38 |
| 128 | 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 |
| 129 | Size Effects on Li<sup>+</sup>/Electron Conductivity in TiO<sub>2</sub> Nanoparticles. Journal of Physical Chemistry Letters, 2010, 1, 1967-1972. | 2.1 | 37 |
| 130 | Molecular structure and free energy landscape for electron transport in the decahaem cytochrome MtrF. Biochemical Society Transactions, 2012, 40, 1198-1203. | 1.6 | 37 |
| 131 | Effect of surface site interactions on potentiometric titration of hematite (Î±-Fe2O3) crystal faces. Journal of Colloid and Interface Science, 2013, 391, 125-134. | 5.0 | 37 |
| 132 | Technetium Stabilization in Low-Solubility Sulfide Phases: A Review. ACS Earth and Space Chemistry, 2018, 2, 532-547. | 1.2 | 36 |
| 133 | Potential docking sites and positions of hydrogen in high-pressure silicates. American Mineralogist, 2003, 88, 1452-1459. | 0.9 | 35 |
| 134 | Molecular dynamics investigation of ferrousâ€“ferric electron transfer in a hydrolyzing aqueous solution: Calculation of the pH dependence of the diabatic transfer barrier and the potential of mean force. Journal of Chemical Physics, 2004, 120, 7607-7615. | 1.2 | 35 |
| 135 | A Connection between Empirical Bond Strength and the Localization of the Electron Density at the Bond Critical Points of the SiO Bonds in Silicates. Journal of Physical Chemistry A, 2004, 108, 7643-7645. | 1.1 | 35 |
| 136 | Experimental Bond Critical Point and Local Energy Density Properties Determined for Mnâˆ’O, Feâˆ’O, and Coâˆ’O Bonded Interactions for Tephroite, Mn2SiO4, Fayalite, Fe2SiO4, and Co2SiO4 Olivine and Selected Organic Metal Complexes: Comparison with Properties Calculated for Non-Transition and Transition Metal Mâˆ’O Bonded Interactions for Silicates and Oxides. Journal of Physical Chemistry A, 2008, 112, 8811-8823. | 1.1 | 35 |
| 137 | Inner-Helmholtz potential development at the hematite (Î±-Fe2O3) (001) surface. Geochimica Et Cosmochimica Acta, 2011, 75, 4113-4124. | 1.6 | 35 |
| 138 | Bonded Radii and the Contraction of the Electron Density of the Oxygen Atom by Bonded Interactions. Journal of Physical Chemistry A, 2013, 117, 1632-1640. | 1.1 | 35 |
| 139 | Automated high-pressure titration system with <i>in situ</i> infrared spectroscopic detection. Review of Scientific Instruments, 2014, 85, 044102. | 0.6 | 35 |
| 140 | The Cs/K Exchange in Muscovite Interlayers: An Ab Initio Treatment. Clays and Clay Minerals, 2001, 49, 500-513. | 0.6 | 34 |
| 141 | Kinetics of Triscarbonato Uranyl Reduction by Aqueous Ferrous Iron:Â A Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 9691-9701. | 1.1 | 34 |
| 142 | Near-infrared spectroscopic investigation of water in supercritical CO2 and the effect of CaCl2. Fluid Phase Equilibria, 2013, 338, 155-163. | 1.4 | 34 |
| 143 | Size dependent microbial oxidation and reduction of magnetite nano- and micro-particles. Scientific Reports, 2016, 6, 30969. | 1.6 | 34 |
| 144 | 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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|---|---|---|---|
| 145 | A Computational Quantum Chemical Study of the Bonded Interactions in Earth Materials and Structurally and Chemically Related Molecules. Reviews in Mineralogy and Geochemistry, 2001, 42, 345-381. | 2.2 | 33 |
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