

# Andrew G Stack

## List of Publications by Year in descending order

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Version: 2024-02-01

84  
papers

2,511  
citations

159585

30  
h-index

233421

45  
g-index

85  
all docs

85  
docs citations

85  
times ranked

2686  
citing authors

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | Accurate Rates of the Complex Mechanisms for Growth and Dissolution of Minerals Using a Combination of Rare-Event Theories. <i>Journal of the American Chemical Society</i> , 2012, 134, 11-14.   | 13.7 | 127       |
| 2  | 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> , 2003, 67, 985-1000. | 3.9  | 125       |
| 3  | 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> , 2013, 47, 205-211.  | 10.0 | 96        |
| 4  | Growth Rate of Calcite Steps As a Function of Aqueous Calcium-to-Carbonate Ratio: Independent Attachment and Detachment of Calcium and Carbonate Ions. <i>Crystal Growth and Design</i> , 2010, 10, 1409-1413.  | 3.0  | 95        |
| 5  | Point of zero charge of a corundum-water interface probed with optical second harmonic generation (SHG) and atomic force microscopy (AFM): New approaches to oxide surface charge. <i>Geochimica Et Cosmochimica Acta</i> , 2001, 65, 3055-3063.                            | 3.9  | 77        |
| 6  | Internal Domains of Natural Porous Media Revealed: Critical Locations for Transport, Storage, and Chemical Reaction. <i>Environmental Science &amp; Technology</i> , 2016, 50, 2811-2829.   | 10.0 | 76        |
| 7  | Interaction force measurement between E. coli cells and nanoparticles immobilized surfaces by using AFM. <i>Colloids and Surfaces B: Biointerfaces</i> , 2011, 82, 316-324.   | 5.0  | 70        |
| 8  | Pore-Size-Dependent Calcium Carbonate Precipitation Controlled by Surface Chemistry. <i>Environmental Science &amp; Technology</i> , 2014, 48, 6177-6183.   | 10.0 | 69        |
| 9  | Calcite Growth Rates As a Function of Aqueous Calcium-to-Carbonate Ratio, Saturation Index, and Inhibitor Concentration: Insight into the Mechanism of Reaction and Poisoning by Strontium. <i>Crystal Growth and Design</i> , 2012, 12, 3540-3548.                         | 3.0  | 66        |
| 10 | Ultra-efficient polymer binder for silicon anode in high-capacity lithium-ion batteries. <i>Nano Energy</i> , 2020, 73, 104804.   | 16.0 | 57        |
| 11 | The dynamic nature of crystal growth in pores. <i>Scientific Reports</i> , 2016, 6, 33086.  | 3.3  | 54        |
| 12 | Growth Kinetics and Morphology of Barite Crystals Derived from Face-Specific Growth Rates. <i>Crystal Growth and Design</i> , 2015, 15, 2064-2071.  | 3.0  | 53        |
| 13 | Heterogeneous Nucleation and Growth of Barium Sulfate at Organicâ€“Water Interfaces: Interplay between Surface Hydrophobicity and Ba <sup>2+</sup> Adsorption. <i>Langmuir</i> , 2016, 32, 5277-5284.   | 3.5  | 53        |
| 14 | Molecular Dynamics Simulations of Solvation and Kink Site Formation at the {001} Bariteâ€“Water Interface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2104-2110.   | 3.1  | 47        |
| 15 | Effect of Strong Acid Functional Groups on Electrode Rise Potential in Capacitive Mixing by Double Layer Expansion. <i>Environmental Science &amp; Technology</i> , 2014, 48, 14041-14048.  | 10.0 | 47        |
| 16 | Adsorption mechanism of alkyl hydroxamic acid onto bastnÃ¡site: Fundamental steps toward rational collector design for rare earth elements. <i>Journal of Colloid and Interface Science</i> , 2019, 553, 210-219.   | 9.4  | 47        |
| 17 | Organicâ€“mineral interfacial chemistry drives heterogeneous nucleation of Sr-rich (Ba <sub>2</sub> SO <sub>4</sub> ) <sub>1-x</sub> (SrSO <sub>4</sub> ) <sub>x</sub> at the National Academy of Sciences of the United States of America, 2019, 116, 13221-13226.         | 7.1  | 45        |
| 18 | Adatom Fe(III) on the hematite surface: Observation of a key reactive surface species. <i>Geochemical Transactions</i> , 2004, 5, 1.  | 0.7  | 44        |

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|----|---|------|-----------|
| 19 | Multi-scale characterization of pore evolution in a combustion metamorphic complex, Hatrurim basin, Israel: Combining (ultra) small-angle neutron scattering and image analysis. <i>Geochimica Et Cosmochimica Acta</i> , 2013, 121, 339-362. | 3.9  | 42        |
| 20 | Upscaling Calcite Growth Rates from the Mesoscale to the Macroscale. <i>Environmental Science &amp; Technology</i> , 2013, 47, 7555-7562.   | 10.0 | 42        |
| 21 | Precipitation in Pores: A Geochemical Frontier. <i>Reviews in Mineralogy and Geochemistry</i> , 2015, 80, 165-190.  | 4.8  | 42        |
| 22 | Extraction of organic compounds from representative shales and the effect on porosity. <i>Journal of Natural Gas Science and Engineering</i> , 2016, 35, 646-660.   | 4.4  | 40        |
| 23 | Solvent-pore interactions in the Eagle Ford shale formation. <i>Fuel</i> , 2019, 238, 298-311.  | 6.4  | 40        |
| 24 | Uncovering the Atomistic Mechanism for Calcite Step Growth. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8464-8467.   | 13.8 | 39        |
| 25 | Direct Imaging of Nanoscale Dissolution of Dicalcium Phosphate Dihydrate by an Organic Ligand: Concentration Matters. <i>Environmental Science &amp; Technology</i> , 2013, 47, 13365-13374.  | 10.0 | 38        |
| 26 | Hydration Structure of the Barite (001)â€“Water Interface: Comparison of X-ray Reflectivity with Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12236-12248.   | 3.1  | 38        |
| 27 | Reaction of hydroquinone with hematite. <i>Journal of Colloid and Interface Science</i> , 2004, 274, 433-441.   | 9.4  | 35        |
| 28 | Structure and Dynamics of Water on Aqueous Barium Ion and the {001} Barite Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 16387-16391.  | 3.1  | 34        |
| 29 | In Situ <sup>27</sup> Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions above and below Saturation with Respect to Gibbsite. <i>Inorganic Chemistry</i> , 2018, 57, 11864-11873.   | 4.0  | 33        |
| 30 | Moving beyond the Solvent-Tip Approximation to Determine Site-Specific Variations of Interfacial Water Structure through 3D Force Microscopy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1282-1291.                                  | 3.1  | 31        |
| 31 | Molecular Dynamics Calculation of the Activation Volume for Water Exchange on Li+. <i>Journal of the American Chemical Society</i> , 2006, 128, 14778-14779.  | 13.7 | 30        |
| 32 | A comparative study of surface energies and water adsorption on Ce-bastnÃ“site, La-bastnÃ“site, and calcite via density functional theory and water adsorption calorimetry. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7820-7832. | 2.8  | 30        |
| 33 | Magnesite Step Growth Rates as a Function of the Aqueous Magnesium:Carbonate Ratio. <i>Crystal Growth and Design</i> , 2014, 14, 6033-6040.   | 3.0  | 28        |
| 34 | Crystal Structures, Surface Stability, and Water Adsorption Energies of La-BastnÃ“site via Density Functional Theory and Experimental Studies. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16767-16781.                               | 3.1  | 28        |
| 35 | Synthesis and structure of synthetically pure and deuterated amorphous (basic) calcium carbonates. <i>Chemical Communications</i> , 2017, 53, 2942-2945.  | 4.1  | 28        |
| 36 | Free-Energy Landscape of the Dissolution of Gibbsite at High pH. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1809-1814.   | 4.6  | 25        |

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|----|---|------|-----------|
| 37 | Effects of Ionic Strength, Salt, and pH on Aggregation of Boehmite Nanocrystals: Tumbler Small-Angle Neutron and X-ray Scattering and Imaging Analysis. <i>Langmuir</i> , 2018, 34, 15839-15853.  | 3.5  | 25        |
| 38 | Reaction of hydroquinone with hematite. <i>Journal of Colloid and Interface Science</i> , 2004, 274, 442-450.   | 9.4  | 24        |
| 39 | Long-Range Electron Transfer across Cytochrome $\text{c}$ –Hematite ( $\text{Fe}_2\text{O}_3$ ) Interfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2096-2103.                        | 3.1  | 24        |
| 40 | Unraveling the Effects of Strontium Incorporation on Barite Growth—In Situ and Ex Situ Observations Using Multiscale Chemical Imaging. <i>Crystal Growth and Design</i> , 2018, 18, 5521-5533.    | 3.0  | 23        |
| 41 | The Growth Morphology of the {100} Surface of KDP (Archerite) on the Molecular Scale. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18284-18290.  | 2.6  | 22        |
| 42 | Pyromorphite Growth on Lead-Sulfide Surfaces. <i>Environmental Science &amp; Technology</i> , 2004, 38, 5529-5534.  | 10.0 | 22        |
| 43 | Simultaneous Adsorption and Incorporation of $\text{Sr}^{2+}$ at the Barite (001)–Water Interface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1194-1207.                                 | 3.1  | 21        |
| 44 | Modeling Water Exchange on an Aluminum Polyoxocation. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23771-23775.  | 2.6  | 20        |
| 45 | Precise determination of water exchanges on a mineral surface. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28819-28828.  | 2.8  | 20        |
| 46 | Molecular Recognition at Mineral Interfaces: Implications for the Beneficiation of Rare Earth Ores. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 16327-16341.                        | 8.0  | 20        |
| 47 | Self-Assembled Monolayers as Templates for Heme Crystallization. <i>Crystal Growth and Design</i> , 2010, 10, 798-805.  | 3.0  | 19        |
| 48 | Investigating calcite growth rates using a quartz crystal microbalance with dissipation (QCM-D). <i>Geochimica Et Cosmochimica Acta</i> , 2018, 222, 269-283.                                     | 3.9  | 19        |
| 49 | Counteractions Control Local Specific Bonding Interactions and Nucleation Mechanisms in Concentrated Water-in-Salt Solutions. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3318-3325. | 4.6  | 19        |
| 50 | Next generation models of carbonate mineral growth and dissolution. , 2014, 4, 278-288.   |      | 18        |
| 51 | Water Uptake by Silica Nanopores: Impacts of Surface Hydrophilicity and Pore Size. <i>Journal of Physical Chemistry C</i> , 2020, 124, 15188-15194.   | 3.1  | 18        |
| 52 | Wellbore Cement Porosity Evolution in Response to Mineral Alteration during CO <sub>2</sub> Flooding. <i>Environmental Science &amp; Technology</i> , 2017, 51, 692-698.                          | 10.0 | 17        |
| 53 | Opposing Effects of Impurity Ion $\text{Sr}^{2+}$ on the Heterogeneous Nucleation and Growth of Barite ( $\text{BaSO}_4$ ). <i>Crystal Growth and Design</i> , 2021, 21, 5828-5839.               | 3.0  | 17        |
| 54 | Adhesion of <i>Shewanella oneidensis</i> MR-1 to Iron (Oxy)(Hydr)Oxides: Microcolony Formation and Isotherm. <i>Environmental Science &amp; Technology</i> , 2010, 44, 1602-1609.                 | 10.0 | 16        |

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|----|---|-----|-----------|
| 55 | Studies of Mineral Nucleation and Growth Across Multiple Scales: Review of the Current State of Research Using the Example of Barite (BaSO <sub>4</sub> ). ACS Earth and Space Chemistry, 2021, 5, 3338-3361.   | 2.7 | 15        |
| 56 | Virtual Probes of Mineral-Water Interfaces: The More Flops, the Better!. Elements, 2013, 9, 211-216.  | 0.5 | 14        |
| 57 | Decoding Oxyanion Aqueous Solvation Structure: A Potassium Nitrate Example at Saturation. Journal of Physical Chemistry B, 2018, 122, 7584-7589.  | 2.6 | 14        |
| 58 | Resolving local configurational contributions to X-ray and neutron radial distribution functions within solutions of concentrated electrolytes – a case study of concentrated NaOH. Physical Chemistry Chemical Physics, 2019, 21, 6828-6838.                   | 2.8 | 14        |
| 59 | Influence of microstructure on replacement and porosity generation during experimental dolomitization of limestones. Geochimica Et Cosmochimica Acta, 2021, 303, 137-158.   | 3.9 | 14        |
| 60 | A Molecular-Scale Approach to Rare-Earth Beneficiation: Thinking Small to Avoid Large Losses. IScience, 2020, 23, 101435.   | 4.1 | 13        |
| 61 | Coupled Multimodal Dynamics of Hydrogen-Containing Ion Networks in Water-Deficient, Sodium Hydroxide-Aluminate Solutions. Journal of Physical Chemistry B, 2018, 122, 12097-12106.  | 2.6 | 12        |
| 62 | Micro-continuum approach for mineral precipitation. Scientific Reports, 2021, 11, 3495.   | 3.3 | 12        |
| 63 | Geochemical reaction mechanism discovery from molecular simulation. Environmental Chemistry, 2015, 12, 20.  | 1.5 | 11        |
| 64 | Chlorite topography and dissolution of the interlayer studied with atomic force microscopy. American Mineralogist, 2014, 99, 128-138.   | 1.9 | 10        |
| 65 | Mineral–Water Interface Structure of Xenotime (YPO <sub>4</sub> ) {100}. Journal of Physical Chemistry C, 2018, 122, 20232-20243.   | 3.1 | 10        |
| 66 | Controls of Microstructure and Chemical Reactivity on the Replacement of Limestone by Fluorite Studied Using Spatially Resolved Small Angle X-ray and Neutron Scattering. ACS Earth and Space Chemistry, 2019, 3, 1998-2016.                                    | 2.7 | 10        |
| 67 | Hydration structure and water exchange kinetics at xenotime–water interfaces: implications for rare earth minerals separation. Physical Chemistry Chemical Physics, 2020, 22, 7719-7727.  | 2.8 | 10        |
| 68 | Grain detachment and transport clogging during mineral dissolution in carbonate rocks with permeable grain boundaries. Geochimica Et Cosmochimica Acta, 2020, 280, 202-220.   | 3.9 | 10        |
| 69 | Dissolution Morphology of Iron (Oxy)(Hydr)Oxides Exposed to the Dissimilatory Iron-Reducing Bacterium <i>Shewanella oneidensis</i> MR-1. Geomicrobiology Journal, 2009, 26, 83-92.  | 2.0 | 9         |
| 70 | Geochemical Evidence for Rare-Earth Element Mobilization during Kaolin Diagenesis. ACS Earth and Space Chemistry, 2018, 2, 506-520.   | 2.7 | 9         |
| 71 | Pb Sorption at the Barite (001)–Water Interface. Journal of Physical Chemistry C, 2020, 124, 22035-22045.   | 3.1 | 9         |
| 72 | Response to comment on “Point of zero charge of a corundum-water interface probed with optical second harmonic generation (SHG) and atomic force microscopy (AFM): new approaches to oxide surface charge”. Geochimica Et Cosmochimica Acta, 2003, 67, 321-322. | 3.9 | 8         |

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|----|---|------|-----------|
| 73 | Local molecular environment drives speciation and reactivity of ion complexes in concentrated salt solution. <i>Journal of Molecular Liquids</i> , 2021, 340, 116898.   | 4.9  | 8         |
| 74 | Molecular Structure of Adsorbed Water Phases in Silica Nanopores. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2885-2895.  | 3.1  | 8         |
| 75 | Radiolysis and Radiation-Driven Dynamics of Boehmite Dissolution Observed by In Situ Liquid-Phase TEM. <i>Environmental Science &amp; Technology</i> , 2022, 56, 5029-5036.                                     | 10.0 | 8         |
| 76 | Solution and Interface Structure and Dynamics in Geochemistry: Gateway to Link Elementary Processes to Mineral Nucleation and Growth. <i>Crystal Growth and Design</i> , 2022, 22, 853-870.                     | 3.0  | 8         |
| 77 | Long-Term <sup>13</sup> C Uptake by <sup>12</sup> C-Enriched Calcite. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 998-1005.   | 2.7  | 7         |
| 78 | Uncovering the Atomistic Mechanism for Calcite Step Growth. <i>Angewandte Chemie</i> , 2017, 129, 8584-8587.  | 2.0  | 6         |
| 79 | Improving Rare-Earth Mineral Separation with Insights from Molecular Recognition: Functionalized Hydroxamic Acid Adsorption onto Bastnaesite and Calcite. <i>Langmuir</i> , 2022, 38, 5439-5453.                | 3.5  | 6         |
| 80 | The "good," the "bad," and the "hidden" in neutron scattering and molecular dynamics of ionic aqueous solutions. <i>Journal of Chemical Physics</i> , 2022, 156, .  | 3.0  | 6         |
| 81 | Numerical Study of Mineral Nucleation and Growth on a Substrate. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 1655-1665.   | 2.7  | 6         |
| 82 | Density Functional Tight-Binding Simulations Reveal the Presence of Surface Defects on the Quartz (101)–Water Interface. <i>Journal of Physical Chemistry C</i> , 2021, 125, 16246-16255.                       | 3.1  | 4         |
| 83 | Frustrated Coulombic and Cation Size Effects on Nanoscale Boehmite Aggregation: A Tumbler Small- and Ultra-Small-Angle Neutron Scattering Study. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4391-4414. | 3.1  | 4         |
| 84 | 5. Precipitation in Pores: A Geochemical Frontier. , 2015, , 165-190.   |      | 1         |