**ANDREW G. STACK**

Group Leader, Geochemistry and Interfacial Sciences
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## Professional Interests

Mineral surface chemistry, particularly nucleation, growth and dissolution. Geochemical reaction kinetics and mechanisms. Reactions in aqueous solutions and porous media. Reactivity of inorganic contaminants.

## Educational Background

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| Ph.D. | Geology | 2002 | University of Wyoming |
| M.S. | Geology | 1999 | University of Wyoming |
| B.S. | Geological Sciences: Geochemistry option | 1997 | Virginia Polytechnic Institute |

## Employment History

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| Group Leader | Oak Ridge National Laboratory | 2017-present |
| Senior R&D Staff | Oak Ridge National Laboratory | 2014-present |
| Acting Division Director | Oak Ridge National Laboratory | 2020-2021, 2017-2018 |
| R&D Staff | Oak Ridge National Laboratory | 2010-2013 |
| Assistant Professor | Georgia Institute of Technology | 2005-2010 |
| Postgraduate Researcher | University of California, Davis | 2002-2005 |
| Graduate Research Assistant | University of Wyoming | 1997-2002 |
| Temporary Scientist Level I | Shepherd-Miller Inc. | 1998 |
| Graduate Teaching Assistant | University of Wyoming | 1997 |
| Hydrologist | U.S. Geological Survey | 1994-1997 |

## Honors & Awards

Outstanding Contributions to Geosciences Research Award (2014). U.S. DOE Basic Energy Sciences, Geosciences Program

Award for One of Top 14 Technical Presentations (out of > 300), Twelfth Annual Conference on Carbon Capture, Utilization & Sequestration. Pittsburgh, PA, May 13-16, (2013)

Finalist for Asylum Research AFM Image Contest (2014)

Profile featured at ORNL web-site (Part I, Part II), STEM Magazine (2015)

Profile featured in American Chemical Society's "College-To-Career" web-site (2014)

ORNL Incentivized Performance Awards (2021, 2020, 2019, 2018, 2016, 2015, 2014)

ORNL Supplemental Performance Awards (2013, 2012, 2011)

Mineralogical Society of America Undergraduate Award (1997)

U.S. Department of Interior On-the-Spot Award (1996)

**Professional Activities and Service**

Member, Basic Energy Sciences Advisory Committee, U.S. Department of Energy, Office of Science (2019-present)

Chair, Committee of Visitors (2020), U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division

Member, Project Science Team, National Alliance for Water Innovation project "Electromagnetic Field for Membrane Scaling Control" (2022-present)

Journal Editorial Board Member, Geochemical Transactions (2013-present)

Faculty Member, Bredesen Center for Interdisciplinary Research and Graduate Education, University Tennessee/Oak Ridge National Laboratory (2016-present)

Member, American Chemical Society National Award Selection Committee (2021-present), Officer, ACS Geochemistry Division: Past Division Chair (2015), Division Chair (2014), Program Chair (2013), Program-Chair Elect (2012), Awards Committee Member (2016-2018). Organizer of Geochemistry Division Programming at National American Chemical Society conferences (fall 2013, spring 2014)

Member of Adjunct Graduate Faculty, Wright State University (2013-2018)

Member of ORNL Committees: Research Conflict of Interest Advisory Committee (2015-2020); Technology Innovation Program Internal Review Committee (2018); Laboratory Directed Research and Development Internal Review Committee, "Next-Generation Techniques and Methods for Neutron Sciences" (2015-2017); Center for Accelerated Materials Modeling Advisory Committee (2015-2016)

Attended Courageous Leaders Summit (2019), Alda-Kavli Leadership Program (2016), ORNL Developing Leadership Potential (2015), and ORNL Management Boot Camp (2013) courses

Co-Organizer of symposia: Semi-annual National American Chemical Society conferences (spring 2020, 2×spring 2015, spring 2014, spring 2013, fall 2013), V. M. Goldschmidt Geochemical Society conferences (2×2015, 2012, 2×2010, 2009, 2007, 2005), Pacifichem (2015)

Member of the Proposal Study Council (2013) & Proposal Study Panel (2012) for the Molecular Foundry, a DOE Nanoscale Science Research Center

Served on U.S. National Science Foundation Geobiology and Low Temperature Aqueous Geochemistry review panels (2012, 2011, 2009)

Served on review panel for the U.S. Department of Energy Biological and Environmental Research Program triennial review of the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory (2011)

Member: *American Chemical Society, American Association for the Advancement of Science*

**Community Workshop Participation**

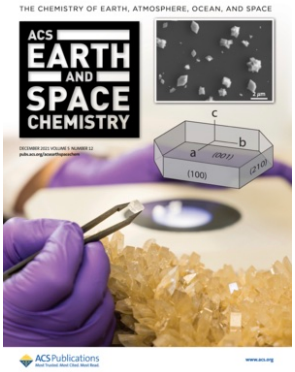
Co-Chair: Subsurface and Geosciences breakout session, AI Town Hall for Science, Lawrence Berkeley National Laboratory (2019)

Panelist and Liaison to the Workshop Chair: Experts' Workshop on Carbon Capture, Utilization and Storage for the Mission Innovation Challenge global initiative (2017)

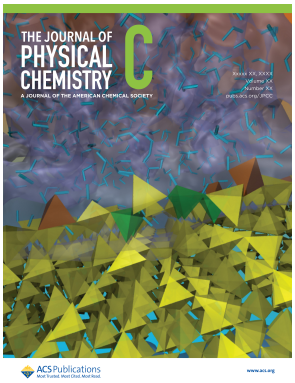
Panelist: Department of Energy, Basic Energy Sciences workshop and contributor to factual document on Basic Research Needs for the Energy-Water Nexus (2017)

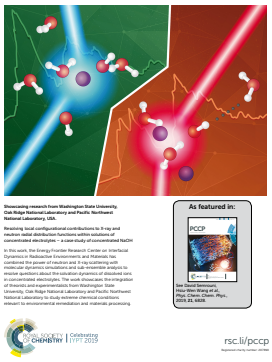
Panelist/Roundtable Expert: Department of Energy, Basic Energy Sciences workshops and contributor to report on Subsurface Technology and Engineering Research Program (SubTER) and a new Grand Challenge for Subsurface Science (2015)

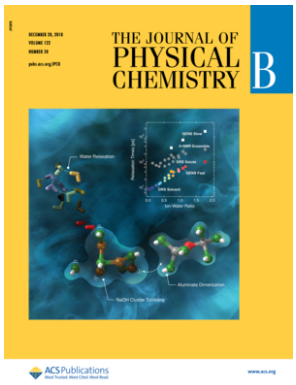
**Journal Covers/Alternate Covers:**

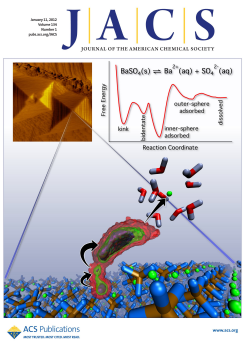





**Publications:** Google H-index = 30. (DOIs are hyperlinks)

1. Weber, J., Starchenko, V., Ilavksy, J. , Allard, L.F., Mata, J., Debeer-Schmitt, L., Cooke, C.G., Littrell, K., He, L., Zhang, R., **Stack, A.G.**, Anovitz, L.M. (2023) Grain Boundary Widening Controls Siderite (FeCO3) Replacement of Limestone ($CaCO_3$). *Sci. Rep.* 13:4581 DOI: 10.1038/s41598-023-30757-y
2. Nakouzi, E.; Kersit, S; Legg, B. A.; Yadav, S.; Li, D.; **Stack, A. G.**; Mundy, C. J.; Chun, J.; Schenter, G. K.; De Yoreo, J. J. (2023) Solution Structure and Hydration Forces between Mica and Hydrophilic Versus Hydrophobic Surfaces. *J. Phys. Chem. C*. 127, 2741-2752. DOI: 10.1021/acs.jpcc.2c09120
3. Roy, S.; Bocharova, V.; **Stack, A. G.**; Bryantsev, V. (2022) Nucleation Rate Theory for Coordination Number: Elucidating Water-Mediated Formation of a Zigzag $Na_2SO_4$ Morphology. *ACS Appl. Mater. Interfaces,* 14, 53213-53227. DOI: 10.1021/acsami.2c17475

4. Brady, A. B.; Weber, J.; Yuan, K.; Allard, L. F.; Avina, O.; Ogaz, R.; Chang, Y.-J.; Rampal, N.; Starchenko, V.; Rother, G.; Anovitz, L. M.; Bañuelos, J. L.; Wang, H.-W.; **Stack, A. G.** (2022) In-Situ Observations of Barium Sulfate Nucleation in Nanopores. *Cryst. Growth Des.,* 22, 6941-6951. DOI: 10.1021/acs.cgd.2c00592
5. Yang, P.; Rampal, N.; Weber, J.; Bracco, J. N.; Fenter, P.; **Stack, A. G.**; Lee, S. S. (2022) Synergistic Enhancement of Lead and Selenate Uptake at the Barite (001)–Water Interface. *Environ. Sci. Technol.,* 56, 16801-16810. DOI: 10.1021/acs.est.2c04413
6. Deng, N.; Zuo, X.; **Stack, A. G.**; Lee, S. S.; Zhou, Z.; Weber, J.; Hu, Y. (2022) Selenite and Selenate Sequestration during Coprecipitation with Barite: Insights from Mineralization Processes of Adsorption, Nucleation and Growth. *Environ. Sci. Technol.,* 56, 15518-15527. DOI: 10.1021/acs.est.2c03292
7. Hajirezaie, S.; Peters, C. A.; Cole, D. R.; Sheets, J. M. Kim, J. J.; Swift, A. M.; Crandall, D.; Cheshire, M. C.; **Stack, A. G**.; Anovitz, L. M. (2022) Sealing fractures to increase underground storage security: Lessons learned from a multiscale multimodal imaging study of a syntaxial vein in a mudrock. *Chem. Geol.,* 614, 121164. DOI: 10.1016/j.chemgeo.2022.121164
8. Nienhuis, E. T.; Pouvreau, M.; Graham, T. R.; Prange, M. P.; Page, K.; Loring, J. S.; **Stack, A. G.**; Clark, A. E.; Schenter, G. K.; Rosso, K. M.; Pearce, C. I.; Wang, H-W. (2022) Structure and reactivity of sodium aluminate complexes in alkaline solutions. *J. Mol. Liq.* 367, 120379. DOI: 10.1016/j.molliq.2022.120379
9. Liu, W.; Pouvreau, M.; **Stack, A. G.**; Yang, X.; Clark, A. E. (2022) Concentration Dependent Interfacial Chemistry of the $NaOH_{(aq)}$:Gibbsite Interface. *Phys. Chem. Chem. Phys.* 56, 5029-5036. DOI: 10.1039/D2CP01997C
10. Page, K.; **Stack, A. G.**; Chen, S. A.; Wang, H.-W. (2022) Nanopore Facilitated Monohydrocalcitic Amorphous Calcium Carbonate Precipitation. *Phys. Chem. Chem. Phys.*, 24, 18340-18346 DOI: 10.1039/d2cp00446a
11. Yang, F.; Yuan, K.; **Stack, A. G.**; Starchenko, V. (2022) Numerical Study of Mineral Nucleation and Growth on a Substrate. *ACS Earth Space Chem.* 6, 1655-1665 DOI: 10.1021/acsearthspacechem.1c00376
12. Biriukov, D.; Wang, H.-W.; Rampal, N.; Tempra, C.; Kula, P.; Neuefeind, J. C.; **Stack, A. G.**; Předota, M. (2022) The "Good", the "Bad", and the "Hidden" in Neutron Scattering and Molecular Dynamics of Ionic Aqueous Solutions. *J. Chem. Phys.* 156, 194505. DOI: 10.1063/5.0093643 Selected as a Feature Article.
13. Chapleski, Jr. R. C.; Chowdhury, A. U.; Wanhala, A. K.; Gibson, L. D.; Stamberga, D.; Janson-Popova, S.; Sacci, R. L.; Meyer, III, H. M.; **Stack, A. G.**; Bocherova, V.; Doughty, B.; Bryantsev, V. S. (2022) Improving Rare-Earth Mineral Separation with Insights from Molecular Recognition: Functionalized Hydroxamic Acid Adsorption onto Bastnäsite and Calcite. *Langmuir,* 38, 5439-5453. DOI: 10.1021/acs.langmuir.1c03422
14. Liu, L.; Chun, J.; Zhang, X.; Sassi, M.; **Stack, A. G.**; Pearce, C. I.; Clark, S. B.; Rosso, K. M.; De Yoreo, J. J.; Kimmel, G. A. (2022) Radiolysis and Radiation-Driven Dynamics of Boehmite Dissolution Observed by In Situ Liquid-Phase TEM. *Environ. Sci Technol.* 56, 8. DOI: 10.1021/acs.est.1c08415

15. Anovitz, L. M.; Huestis, P.; Rampal, N.; **Stack, A. G.**; LaVerne, J. A.; Zhang, X.; Schenter, G. K.; Chun, J.; Legg, B. A.; Liu, L.; Bleuel, M.; Gagnon, C.; Mildner, D. F. R. (2022) Frustrated Coulombic and Cation Size Effects on Nanoscale Boehmite Aggregation: A Tumbler Small- and Ultra-Small Angle Neutron Scattering Study. *J. Chem. Phys. C* 126, 4391-4414. DOI: 10.1021/acs.jpcc.1c10580
16. Rother, G.; Gautam, S.; Liu, T.; Cole, D. R.; Busch, A.; **Stack, A. G.** (2022) Molecular Structure of Adsorbed Water Phases in Silica Nanopores. *J. Phys. Chem. C* 126, 2885-2895 DOI: 10.1021/acs.jpcc.1c10162
17. Wang, H.-W.; Yuan, K.; Rampal, N.; **Stack, A. G.** (2021) Solution and Interface Structure and Dynamics in Geochemistry: Gateway to Link Elementary Processes to Mineral Nucleation and Growth. *Cryst. Growth Des.* 22, 852-870 DOI: 10.1021/acs.cgd.1c00563
18. Weber, J.; Bracco, J. N.; Yuan, K.; Starchenko, V.; **Stack, A. G.** (2021) Studies of Mineral Nucleation and Growth Across Multiple Scales: Review of the Current State of Research using the example of Barite ($BaSO_4$). *ACS Earth Space Chem.* 5, 3338-3361 DOI: 10.1021/acsearthspacechem.1c00055
19. Yuan, K.; Starchenko, V.; Rampal, N.; Yang, F.; Yang, X.; Lee, W.-K.; **Stack, A. G.** (2021) Opposing effects of impurity ion $Sr^{2+}$ on the heterogeneous nucleation and growth of barite ($BaSO_4$). *Cryst. Growth Des.,* 21, 5828-5839 DOI: 10.1021/acs.cgd.1c00715
20. **Stack, A. G.**; Wang, H.-W.; Cole, D. R. (2021) Nano-Scale Structure and Dynamics in Geochemical Systems. *Elements* 17, 169-174, DOI: 10.2138/gselements.17.3.169
21. Yuan, K.; Rampal, N.; Fenter, P.; Kubicki, J.; **Stack, A. G.**; Irle, S. (2021) Density Functional Tight-Binding Simulations Reveal the Presence of Surface Defects on the Quartz (101)-Water Interface. *J. Phys. Chem. C, 125*, 16246-16255 DOI: DOI: 10.1021/acs.jpcc.1c03689.
22. Rampal, N.; Wang, H.-W.; Biriukov, D.; Brady, A. B.; Neuefeind, J. C.; Předota, M.; **Stack, A. G.** (2021) Local molecular environment drives speciation and reactivity of ion complexes in concentrated salt solution. *J. Mol. Liq.* 340, 116898 DOI: 10.1016/j.molliq.2021.116898
23. Géhin, A.; Gilbert, B.; Chakraborty, S.; **Stack, A. G.**; Allard, L. F.; Robinet, J.-C.; Charlet, L. (2021) Long-term $^{13}C$ Uptake by $^{12}C$-enriched Calcite. *ACS Earth Space Chem.,* 5, 998-1005 DOI:10.1021/acsearthspacechem.0c00122
24. Weber, J.; Cheshire, M. C.; Bleuel, M.; Mildner, D.; Chang, Y. J.; Ievlev, A.; Littrel, K. C.; Ilavsky, J.; **Stack, A. G.**; Anovitz, L. M. (2021) Influence of Microstructure on Replacement and Porosity Generation during Experimental Dolomitization of Limestones. *Geochim. Cosmochim. Acta*, 303, 137-158. DOI: 10.1016/j.gca.2021.03.029
25. Yang, F.; **Stack, A. G.**; Starchenko, V. (2021) Micro-continuum Approach to Mineral Precipitation: Application to Barite Formation. *Sci. Rep.*, 11, 1-14. DOI: 10.1038/s41598-021-82807-y
26. Nakouzi, E.; **Stack, A. G.**; Kerisit, S.; Legg, B.; Mundy, C.; Schenter, G.; Chun, J.; De Yoreo, J. J. (2021) Moving beyond the Solvent-Tip Approximation to Determine Site-

Specific Variations of Interfacial Water Structure through 3D Force Microscopy. *J. Phys. Chem. C,* 125, 1282-1291. DOI: 10.1021/acs.jpcc.0c07901

27. Bracco, J. N.; Lee, S. S.; Braha, I.; Dorfman, A.; Fenter, P.; **Stack, A. G.** (2020) Pb Sorption at the Barite (001)-Water Interface. *J. Phys. Chem. C,* 124, 22035-22045
28. Chapelski, Jr., R. C.; Chowdhury, A. U.; Wanhala, A. K.; Bocharova, V.; Roy, S; Keller, P. C.; Everly, D.; Jansone-Popova, S.; Kisliuk, A.; Sacci, R. L.; **Stack, A. G.**; Anderson, C. G.; Doughty, B.; Bryantsev, V. S. (2020) A Molecular-Scale Approach to Rare-Earth Beneficiation: Thinking Small to Avoid Large Losses. *iScience*, 101435. DOI: 10.1016/j.isci.2020.101435
29. Rother, G.; **Stack, A. G.**; Gautam, S. S.; Liu, T.; Cole, D. R.; Busch, A. (2020) Water Uptake by Silica Nanopores: Impacts of Surface Hydrophilicity and Pore Size. *J. Phys. Chem. C,* 124, 15188-15194. DOI: 10.1021/acs.jpcc.0c02595
30. Liu, M.; Starchenko, V.; Anovitz, L. M.; **Stack, A. G.** (2020) Grain detachment and transport clogging during mineral dissolution in carbonate rocks with permeable grain boundaries. *Geochim. Cosmochim. Acta*, 280, 202-220. DOI: 10.1016/j.gca.2020.04.022
31. Gao, S.; Sun, F.; Brady, A.; Pan, Y.; Erwin, A.; Yang, D.; Truskruk, V.; **Stack, A. G.**; Saito, T.; Yang, H.; Cao, P.-F. (2020) Ultra-efficient polymer binder for silicon anode in high-capacity lithium-ion batteries. *Nano Energy*, 73, 104804 DOI: 10.1016/j.nanoen.2020.104804
32. Roy, S.; Wu, L.; Srinivasan, S. G.; **Stack, A. G.**; Navrotsky, A.; Bryantsev, V. S. (2020) Hydration structure and water exchange kinetics at xenotime–water interfaces: implications for rare earth minerals separation. *Phys. Chem. Chem. Phys.* 22, 7719-7727 DOI: 10.1039/D0CP00087F
33. Sutton, J. E.; Roy, S.; Chowdhury, A. U.; Wu, L.; Wanhala, A. K.; De Silva, N.; Jansone-Popova, S.; Hay, B. P.; Cheshire, M. C.; Windus, T. L.; **Stack, A. G.**; Navrotsky, A.; Moyer, B. A.; Doughty, B.; Bryantsev, V. S. (2020) Molecular Recognition at Mineral Interfaces: Implications for the Beneficiation of Rare Earth Ores. *ACS Appl. Mater. Int.* 12, 16327-16341. DOI: 10.1021/acsami.9b22902
34. Weber, J.; Cheshire, M. C.; DiStefano, V. H.; Littrell, K. C.; Ilavsky, J.; Bleuel, M.; Bozell-Messerschmidt, J. K.; Ievlev, A.; **Stack, A. G.**; Anovitz, L. M. (2019) 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 Space Chem.* 3, 1998-2016 DOI: 10.1021/acsearthspacechem.9b00085
35. Wanhala, A. K.; Doughty, B. Bryantsev, V. S.; Wu, L.; Mahurin, S. M.; Jansone-Popova S.; Cheshire, M. C.; Navrotsky, A.; **Stack, A. G.** (2019) Adsorption Mechanism of Alkyl Hydroxamic Acid onto Bastnäsite: Fundamental Steps toward Rational Collector Design for Rare Earth Elements. *J. Coll. Int. Sci.* 553, 210-219, DOI: 10.1016/j.jcis.2019.06.025
36. Wang, H.-W.; Graham, T. R.; Mamontov, E.; Page, K.; **Stack, A. G**.; Pearce, C. I. (2019) Countercations Control Local Specific Bonding Interactions and Nucleation Mechanisms in Concentrated Water-in-Salt Solutions. *J. Phys. Chem. Lett.* 10, 3318-3325, DOI: 10.1021/acs.jpclett.9b01416
37. Deng, N.; **Stack, A. G.**; Weber, J.; Cao, B.; De Yoreo, J. J.; Hu, Y. (2019) Organic–mineral interfacial chemistry drives heterogeneous nucleation of Sr-rich $(Ba_x, Sr_{1-x})SO_4$ from

undersaturated solution. *Proc. Nat'l. Acad. Sci.* 116, 13221-13226, DOI: 10.1073/pnas.1821065116

38. Semrouni, D.; Wang, W.-H.; Clark, S. B.; Pearce, C.; Page, K.; Schenter, G.; Wesolowski, D. J.; **Stack, A. G.**; Clark, A. E. (2019) Resolving local configurational contributions to X-ray and neutron radial distribution functions within solutions of concentrated electrolytes – a case study of concentrated NaOH. *Phys. Chem. Chem. Phys.* 21, 6828-6838 DOI: 10.1039/c8cp06802j
39. DiStefano, V. H.; McFarlane, J.; **Stack, A. G.**; Perfect, E.; Mildner, D. F. R.; Bleuel, M.; Chipera, S. J.; Littrell, K. C.; Cheshire, M. C.; Manz, K. E.; Anovitz, L. M. (2019) Solvent-pore interactions in the Eagle Ford shale formation. *Fuel*, 238, 298-311. DOI: 10.1016/j.fuel.2018.10.010
40. Bracco, J. N.; Lee, S. S.; Stubbs, J. E.; Eng, P. J.; Jinda, S.; Warren, D. M.; Kommu, A.; Fenter, P.; Kubicki, J. D.; **Stack, A. G.** (2019) Simultaneous Adsorption and Incorporation of $Sr^{2+}$ at the Barite (001) – Water Interface. *J. Phys. Chem. C* 123, 1194-1207 DOI: 10.1021/acs.jpcc.8b08848
41. Graham, T. R.; Semrouni, D.; Mamontov, E.; Ramirez-Cuesta, A. J.; Page, K.; Clark, A. E.; Schenter, G. K.; Pearce, C. I.; **Stack, A. G.**; Wang, H-W. (2018) Coupled Multimodal Dynamics of Hydrogen-Containing Ion Networks in Water-Deficient, Sodium-Hydroxide-Aluminate Solutions. *J. Phys. Chem. B* 122, 12097-12106, DOI:10.1021/acs.jpcb.8b09375
42. Anovitz, L. M.; Zhang, X.; Soltis J.; Nakouzi, E.; Krzysko, A. J.; Chun, J.; Schenter, G. K.; Graham, T. R.; Rosso, K. M.; De Yoreo, J. J.; **Stack, A. G.**; Bleuel, M.; Gagnon, C.; Mildner, D. F. R.; Ilavsky, J.; Kuzmenko, I. (2018) Effects of Ionic Strength, Salt, and pH on Aggregation of Boehmite Nanocrystals: Tumbler Small-Angle Neutron and X-ray Scattering and Imaging Analysis. *Langmuir 34*, 15839-15853 DOI: 10.1021/acs.langmuir.8b00865
43. **Stack, A. G.**; Stubbs, J. E.; Srinivasan, S. G.; Roy, S.; Bryantsev, V. S.; Eng, P. J.; Custelcean, R.; Gordon, A. D.; Hexel, C. R. (2018) Mineral-Water Interface Structure of Xenotime ($YPO_4$) {100} *J. Phys. Chem. C* 122, 20232-20243 DOI:10.1021/acs.jpcc.8b04015
44. Weber, J.; Bracco, J. N.; Poplawsky, J. D.; Ievlev, A.; More, K. L.; Lorenz, M.; Bertagni, A. L.; Jindra, S. A.; Starchenko, V.; Higgins, S. R.; **Stack, A. G.** (2018) Unraveling the Effects of Strontium Incorporation on Barite Growth – In-situ and Ex-situ Observations using Multi-Scale Chemical Imaging. *Cryst. Growth Des.* 18, 5521-5533 DOI: 10.1021/acs.cgd.8b00839
45. Wang, H.-W.; Vlcek, L.; Neuefeind, J.; Page, K.; Irle, S.; Simonson, J. S.; **Stack, A. G.** (2018) Decoding Oxyanion Aqueous Solvation Structure: A Potassium-Nitrate Example at Saturation. *J. Phys. Chem. B.* 122, 7584-7589 DOI: 10.1021/acs.jpcb.8b05895
46. Graham, T. R.; Dembowski, M.; Martinez-Baez, E.; Zhang, X.; Jaegers, N. R.; Hu, J.; Gruskiewicz, M. S.; Wang, H.-W.; **Stack, A. G.**; Bowden, M. E.; Delegard, C. H.; Schenter, G. K.; Clark, A. E.; Clark, S. B.; Felmy, A. R.; Rosso, K. M.; Pearce, C. I. (2018) In-Situ $^{27}Al$ NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions

Above and Below Saturation with Respect to Gibbsite. *Inorg. Chem. 57,* 11864-11873 DOI: 10.1021/acs.inorgchem.8b00617

47. Cheshire, M. C.; Bish, D. L.; Cahil, J. F.; Kertesz, V.; **Stack, A. G.** (2018) Geochemical evidence for rare-earth element mobilization during kaolin diagenesis. *ACS Earth Space Chem.* 2*,* 503-520 DOI: 10.1021/acsearthspacechem.7b00124
48. Shen, Z.; Kerisit, S.; **Stack, A. G.**; Rosso, K. M. (2018) Free-Energy Landscape of the Dissolution of Gibbsite at High pH. *J. Phys. Chem. Lett.* 9, 1809-1814. DOI: 10.1021/acs.jpclett.8b00484
49. Cao, B.; **Stack, A. G.**; Steefel, C. I.; DePaolo, D. J.; Lammers, L. N.; Hu, Y. (2018) Investigating Calcite Growth Rates Using a Quartz Crystal Microbalance with Dissipation (QCM-D). *Geochim. Cosmochim. Acta 222*, 269-283. **DOI:** 10.1016/j.gca.2017.10.020
50. Bracco, J. N.; Lee, S. S.; Stubbs, J. E.; Eng, P. J.; Heberling, F.; Fenter, P.; **Stack, A. G.** (2017) Hydration Structure of the Barite (001)-Water Interface: Comparison of X-ray Reflectivity with Molecular Dynamics Simulations. *J. Phys. Chem. C 122*, 12236-12248 DOI: 10.1021/acs.jpcc.7b02943
51. De La Pierre, M.; Raiteri, A. G.; **Stack, A. G.**; Gale, J. D. (2017) Uncovering the atomistic mechanism for calcite step growth. *Angew. Chem. Int'l. Ed. 56*, 8464-8467 DOI: 10.1002/ange.201701701
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Adsorption Energies of La-Bastnäsite via Density Functional Theory and Experimental Studies. *J. Phys. Chem. C*, 120, 2811-2829, DOI: 10.1021/acs.jpcc.6b04747

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62. Godinho, J. R. A.; **Stack, A. G.** (2015) Growth kinetics and morphology of barite crystals derived from face-specific growth rates. *Cryst. Growth Des.* 15, 2064-2071 DOI: 10.1021/cg501507p
63. **Stack, A. G.**; Kent, P. R. C. (2015) Geochemical Reaction Mechanism Discovery from Molecular Simulation. *Environ. Chem.* 12, 20-32. DOI: 10.1071/EN14045
64. Hatzell, M. C.; Raju, M.; Watson, V. J.; **Stack, A. G.**; van Duin, A. C. T.; Logan, B. E. (2014) Effect of Strong Acid Functional Groups on Electrode Rise Potential in Capacitive Mixing by Double Layer Expansion. *Environ. Sci. Technol.* 48, 14041-14048. DOI: 10.1021/es5043782
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85. **Stack A. G.**, Rustad J. R., Casey W. H. (2005) Modeling water exchange on an aluminum polyoxocation. *J. Phys. Chem. B* (Letters) **109**, pp. 23771-23775.

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88. **Stack A. G.**, Eggleston C. M. & Engelhard M. H. (2004) Reaction of hydroquinone with hematite I: Electrochemical scanning tunneling microscopy and X-ray photoelectron spectroscopy. *J. Coll. Int. Sci.,* **274**, pp. 433-441.
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**Research Grants and Contracts**

"Mechanisms of Atomic- to Pore-Scale Geochemical Processes." (ERKCC72) U.S. DOE, Office of Basic Energy Sciences (2010-2022) $2,000k/yr. 6 person-months per year. Principal Investigator & Thrust 1 Leader (2015-present); Subtask 2 Leader (2012-2015); Subtask 1 Leader (2010-2012).

**“**Fundamental Mechanisms Driving Efficiency of $CO_2$ Capture Using Mineral Looping” (ERKCK59) U.S. DOE, Office of Basic Energy Sciences (2022-2025) $1,500k/yr. 3 person-months per year. Team Member (2022-present).

“IDREAM: Interfacial Dynamics in Radioactive Environments and Materials.” (ERKCG08) Energy Frontier Research Center funded by the U.S. DOE, Office of Basic Energy Sciences (2016-2024) $3,500k/yr (ORNL portion $400k/yr tentative). 3 person-months per year. Science Thrust 3 Leader (2020-present); ORNL Point of Contact and Leadership Team member (2016-present).

“Direct Air Capture of $CO_2$ Using Mineral Looping” (LOIS10965) ORNL Laboratory Directed Research and Development. (2022) $250k/yr. 3 person-months per year. Principal Investigator.

“Center for Nanoscale Control of Geologic $CO_2$” (ERKCC67) Energy Frontier Research Center, U.S. DOE, Office of Basic Energy Sciences (2014-2018) $3,200k/yr (ORNL portion $490k/yr). 3 person-months per year. ORNL Team Lead (2013-2019),Team Member (2010-2013).

“Critical Materials Institute.” (CEED500) Energy Innovation Hub, U.S. DOE, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office. (2013-2021). Project 1.1.12 Team Member (2018-present), Project 1.1.1 Team Leader (2015-2018); Project 1.1.1 Team Member (2013-2015).

“Reducing Environmental Impacts of Hydrofracturing by Subsurface Co-Precipitation of Barium and Radium.” (LOIS6735) ORNL Laboratory Directed Research and Development. $388k/yr. 03/15/13 - 03/14/15. 2 person-months per year. Principal Investigator (2013-2015).

“Improving Chemical Separations through Understanding Weak Interactions” (ERKCC51) U.S. DOE, Office of Basic Energy Sciences, 8/1/12 – 7/31/15, $400k/yr. 2 person-months per year. Team Member (2012-2015).

“Testing Molecular Mechanisms for Growth and Dissolution Reactions on Calcite Surfaces” (Award #0643139) U.S. NSF, Earth Sciences Directorate, Geobiology and Low Temperature Aqueous Geochemistry program, (2007-2010), $219,385. Principal Investigator.

“Reaction mechanisms for barite dissolution and growth.” (DE-FG02-07ER15901) U.S. DOE, Basic Energy Sciences Program, Geosciences Subprogram, (2007-2009), $209,747. Principal Investigator.

“Characterization of Mineral Dust Aerosols to Improve Predictions of Their Impact on the Radiative Balance of the Atmosphere.” U.S. NOAA, (2007-2010), $314,741. Co-Investigator.

**Invited Talks and Symposia**

1. “Precipitation in nanopores: Sources and magnitudes of anomalous reactivity” *ACS Spring National Meeting in San Diego, California & Virtual*, March, 20-24, 2022
2. “Precipitation in nanopores: Anomalous reactivity” *U.S. DOE Basic Energy Sciences, Geosciences Program*, *Research PI Meeting*, August 4-6th, 2021

3. "Mineral Precipitation from the Atomic to Pore-Scales" *University of Tennessee, Department of Earth and Planetary Sciences.* On-line, April 8th, 2021
4. "Measurements of Concentrated Aqueous Solution Structures and Implications for Nucleation." *Goldschmidt 2020 Workshop : Crystallization via non-classical pathways.* On-line, June 21, 2020.
5. "Solvation Structure and Ion Complex Reactivity in Concentrated Aqueous Salt Solutions." *V. M. Goldschmidt Conference*, on-line, June 22, 2020.
6. "Atomic-Level Fluid Structure and Dynamics for X-ray and Neutron Scattering." *Guest Lecture for Graduate Level Princeton Course: "Synchrotron and neutron techniques for energy materials"*, April 27, 2020
7. "Calcite and Barite Mineral Precipitation in (Nano)Porous Media." *257th ACS National Meeting in Orlando, Florida*, March 31-April 4, 2019.
8. "Linking computational simulation with neutron diffraction to understand ion solvation structure and ion pairing in aqueous solutions. *255th ACS National Meeting in New Orleans, Louisiana,* March 18-22, 2018.
9. "Atomic-to pore-scale geochemistry: Effects of ion sorption and incorporation on mineral growth." *255th ACS National Meeting in New Orleans, Louisiana,* March 18-22, 2018.
10. "Insights into Geochemical Transformations Probed by Examining Solution and Solid Phase Structures Using Neutron Diffraction and Atomic-Scale Simulation." *U.S. DOE Basic Energy Sciences, Geosciences Program*, *Research PI Meeting*, August 7-8th, 2017.
11. "Quasi-Elastic Neutron Scattering Measured on a Mineral-Water Interface, Coupled to Process-Based Mineral Crystal Growth Models." *Oak Ridge National Laboratory, Joint Nanoscience and Neutron Scattering User Meeting*. August 1-2nd, 2017.
12. "Atomic- to Pore-Scale Probes of Mineral Reactivity in Subsurface Environments." *Brookhaven National Laboratory*, workshop on "*Synchrotron Techniques in Support of DOE's Subsurface R&D Effort.*" May 15-16th, 2017.
13. "Mineral Precipitation Reactions from the Atomic- to Pore-Scales." Departmental Seminar. *University of Delaware, Department of Geological Sciences.* May 4th, 2017.
14. "Atoms to pores concepts for mineral growth and precipitation." Session on "Geochemistry Division Medal: Symposium in Honor of Dr. Susan Brantley." *253rd ACS National Meeting in San Francisco, California,* April 2-6, 2017.
15. "Fast solvent exchange on a mineral-water interface coupled to process-based mineral precipitation models." Session on "Mineral-Water Interface Chemistry." *253rd ACS National Meeting in San Francisco, California,* April 2-6, 2017.
16. "Carbonation reactions and their effect on pore distributions in a cement exposed to $CO_2$ for $30^+$ years." Session on "Pore-Scale Geochemical Processes & The Implications for $CO_2$ Geologic Storage." *253rd ACS National Meeting in San Francisco, California,* April 2-6, 2017. Also selected to be presented as a Sci-Mix poster.

17. "Towards a Fundamental Understanding of the Evolution of Porosity and Permeability During Mineral Nucleation and Growth" *American Geophysical Union Fall Meeting*, San Francisco, CA, December 12, 2016.
18. "Towards a fundamental understanding of the nucleation and growth of minerals in porous media." *U.S. DOE Basic Energy Sciences, Geosciences Program*, Research PI Meeting, August 15-16, 2016.
19. "Mineral Precipitation Reactions from the Atomic to Pore Scales" Departmental Seminar, *Institut des Sciences de la Terre, Centre National de la Recherche Scientifique/ Académie Grenoble*, Grenoble, France, Jan. 11, 2016.
20. "Mineral Precipitation Reactions from the Atomic- to Pore Scales." Departmental Colloquium, *Pennsylvania State University, Department of Geosciences*, Oct. 6, 2015.
21. "Precipitation in Pores" Keynote address in session "Pore Scale and Nano-Confined Geochemical Processes," *V. M. Goldschmidt Conference*, Aug., 20, 2015.
22. "Precipitation in Pores: A Geochemical Frontier" Short Course Lecture, *Reviews in Mineralogy and Geochemistry*, Volume 80, "Pore-Scale Geochemical Processes." Aug. 15, 2015.
23. "Atomic- to Pore-Scale Understanding and Prediction of Mineral Precipitation." Departmental seminar, *University of Houston, Dept. of Civil and Environ. Engineering*. Nov. 24, 2014.
24. "Atomic- to Pore-Scale Probes and Predictions of Mineral Reactivity." *U.S. DOE Basic Energy Sciences, Geosciences Program*, Research PI Meeting, May 14-16, 2014.
25. "Atomic-scale to Mesoscale simulation of mineral growth and dissolution reactions." *247th Meeting of the American Chemical Society*, Dallas, TX, March 16-20, 2014.
26. "Mechanisms and Rates of Reaction for Crystallization from the Atomic to Macroscopic Scales: Simulation, Theory and Experiment." *Advanced Photon Source User Seminar Series*, Nov. 15, 2013.
27. "Upscaling Carbonate Mineral Growth Rates From the Nano- to Pore- Scales and Beyond: Current Progress and Future Directions." *Twelfth Annual Conference on Carbon Capture, Utilization & Sequestration.* Pittsburgh, PA, May 13-16, 2013.
28. "Mechanisms and Rates of Reaction at Mineral-Water Interfaces from the Atomic to Pore Scales: Simulation, Theory and Experiment." *Division Seminar, Chemical Sciences and Materials Sciences Divisions, ORNL*. April 17, 2013.
29. "Fast Water Exchange on a Mineral Surface Measured by Quasi-Elastic Neutron Scattering (QENS) and Classical Molecular Dynamics (MD)." Session on "Approaching the Surface: Interrogating Chemical Interactions at the Mineral-Water Interface.' *245th Meeting of the American Chemical Society*, New Orleans, LA, April 7-11, 2013
30. "Nucleation and Growth of Minerals (Calcium Carbonate) in Porous Media" *U.S. DOE BES Geosciences Workshop* on "Reaction and Transport within Internal Domains of Porous Media" San Francisco, December 1-2, 2012.

31. “Calcite Growth from the Molecular Scale.” Session on Physicochemical constraints of the marine carbonate system: recent insights into the reactivity of carbonate minerals in aqueous solutions. *Goldschmidt 2012*, Montréal, Canada, June 24-29, 2012.
32. “Molecular level mechanisms of mineral growth and dissolution.” *Seminar for Geophysical Laboratory*. *Carnegie Institute*, Washington, D. C., January 9, 2012.
33. "Rates of mineral growth and dissolution reactions from molecular dynamics." Session on Large and Complex Atomistic Systems: Physics, Algorithms and Hardware. *Goldschmidt 2011*, Prague, Czech Republic, August 14-19, 2011.
34. “Interaction between iron respiring bacteria and iron (oxy)(hydr)oxides.” Departmental seminar at *Washington University at St. Louis*, Department of Earth and Planetary Sciences. September 17, 2009.
35. "Reactions controlling step movement during mineral dissolution and growth" Session on Molecular Computational Geochemistry for Water-Rock Interactions. *237th Meeting of the American Chemical Society*, Salt Lake City, March 22-26, 2009
36. “Applications of electrochemical scanning tunneling microscopy to adsorption and thin films in geochemical systems.” Session on Advanced Approaches to investigating Adsorption at the solid–Water interface., *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008
37. “Comparison of computational and experimental barite-water interface structures and kinetics.” Session on Physical chemistry of environmental interfaces. *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008
38. “Water structure on aqueous ions and barite-water interfaces.” Division of Colloid and Surface Chemistry. *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008.
39. “Prediction of ligand exchange and crystal growth kinetics using atomistic computational methods. Seminar. *William R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory*. Richland, WA, January 14th, 2008.
40. “Modeling water exchange on an aluminum polyoxocation.” Seminar. *Chemical and Analytical Sciences Division, Oak Ridge National Laboratory*. Oak Ridge, TN, October 10th, 2005.

**Graduate Student and Post-Doctoral Advisees**

Oak Ridge National Laboratory

Dr. Tingting Liu, Post-Doctoral Researcher (2022-present)

Dr. Athena Chen, Post-Doctoral Researcher (2022-present)

Mr. Nikhil Rampal, Columbia Univ. Ph.D. Student, through ORNL-Columbia MOU (2018-2022). Currently a post-doc at Lawrence Livermore Nat’l. Lab.

Dr. Alexander (Sandy) Brady, Post-Doctoral Researcher (2018-2021). Currently an Application Engineer, Bruker Corporation

Dr. Fengchang Yang, Post-Doctoral Researcher (2019-2021). Currently an Associate Professor, Chinese Academy of Sciences

Dr. Ke Yuan, post-doctoral researcher (2019-2020) Currently an R&D Staff Associate, ORNL
Dr. Anna Wanhala, Bredesen Center Ph.D. Student (2015-2020) Currently a post-doc, U. Chicago
Dr. Juliane Weber, Post-Doctoral Researcher (2017-2019) Currently an R&D Staff Associate, ORNL
Dr. Min Liu, Post-Doctoral Researcher (2018-2019) Currently a post-doc, U. Minnesota
Dr. Hsiu-Wen Wang, UTK-ORNL Joint Institute for Neutron Scattering Researcher (2014-2018)
Dr. Michael C. Cheshire, Post-Doctoral Researcher (2014-2016) Currently Staff, Chevron
Dr. José R. A. Godinho, Post-Doctoral Researcher (2013-2015) Currently a Research Scientist, Helmholtz-Zentrum Dresden-Rossendorf
Dr. Alexander D. Gordon, Post-Doctoral Researcher (2013-2014) Currently Staff, Signature Science

Georgia Institute of Technology
Dr. Jacquelyn N. Bracco, undergraduate & M.S. student (2012) Currently Ass't. Prof., CUNY-Queens College. (Received NSF CAREER award in 2021!)
Mr. Davis "Morgan" Warren, M.S. student (2011)
Ms. Cynthia M. Jackson, undergraduate student (2011)
Dr. Mengni Zhang, Ph.D. (Received departmental best paper award, 2009; graduated fall, 2010) Currently an Environmental Scientist, NewFields, Inc.
Dr. Xuefeng Wang, postdoctoral researcher (2008-2010) Currently a Ph.D. Fellow, Seattle Children's Hospital
Ms. Lindsay Wallace, non-thesis MS. (2010) Currently an Environmental Scientist, NewFields, Inc.

**Academic Committee Service**

Dissertation & Thesis Committee Membership
Samuel Evans, Ph.D. University of Tennessee, Knoxville (summer 2019)
Victoria DiStefano, Ph.D., University of Tennessee, Knoxville (summer, 2018), currently at U.S. Dept. of Energy, Office of Science
Chong Dai, Ph.D., University of Houston (spring 2018), currently a post-doc at Rice Univ.
Jacquelyn N. Bracco, Ph.D., Wright State University (fall 2015), currently Prof. at CUNY
Dennis Lenaerts, M.S., Wright State University (spring 2013)

Department Committee Membership - Georgia Institute of Technology
Co-Chair, Graduate Student Acceptance Committee (2009/2010)
Graduate Student Acceptance Committee (2005-2009)
Undergraduate Curriculum Committee (2006/2007)
EAS Faculty Search Committee (2006/2007)
Multiple Graduate Student Thesis Committees (2005-2010)

**Teaching Experience**

Georgia Institute of Technology, School of Earth and Atmospheric Sciences

| **Semester** | **Course** | **Title** | **Enrollment** |
|---|---|---|---|

| | | | |
|---|---|---|---|
| Spring, 2010 | 8803 (Grad) | Special Study: The Origin of Life | 1 |
| Fall, 2009 | 4110 (U.Grad) | Resources, Energy and the Environment | 20 |
| Fall, 2009 | 8803 (Grad) | Mineral Surface Geochemistry | 10 |
| Fall, 2009 | 4900 (U.Grad) | Special Study: C++ for Geochemists | 3 |
| Fall, 2008 | 4803/8803 (U.Grad/Grad) | Resources, Energy and the Environment | 28 |
| Spring, 2008 | 4803/8803 (U.Grad/Grad) | Water Quality Modeling | 4 |
| Fall, 2007 | 4803 (U.Grad) | Resources, Energy and the Environment | 18 |
| Spring, 2007 | 4803/8803 (U.Grad/Grad) | Water Quality Modeling | 5 |
| Fall, 2006 | 8803 (Grad) | Mineral Surface Geochemistry | 9 |
| Fall, 2005 | 4803/8803 (U.Grad/Grad) | Water Quality Modeling | 5 |

University of Wyoming, Department of Geology and Geophysics

| **Semester** | **Course** | **Title** | **Enrollment** |
|---|---|---|---|
| Summer, 2001 | GEOL/ASTR 1070 | The Earth: Its Physical Environment | 6 |

(U. Wyo. Wind River Reservation Extension)

Teaching Assistantships:

| | | |
|---|---|---|
| 1999-2002 | U. Wyo. | The Earth: Its Physical Environment |
| 1997 | U. Wyo. | Physical Geology |
| 1997 | VPI | General Chemistry |