Xin Gu

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Education

2012–2017 **PhD in geosciences and biogeochemistry**, *Department of Geosciences, Pennsylvania State University*, University Park, PA.

Dissertation Characterizing structure and geochemistry of shale pores by neutron scattering

Advisor Susan L. Brantley

2009–2011 **Master of Science**, *School of Forest Resources, Pennsylvania State University*, University Park, PA.

2005–2008 **Master of Science**, *Research Center for Eco-Environmental Science, Chinese Academy of Science*, Beijing, China.

2000–2004 **Bachelor of Engineering**, *Department of Environmental Science and Engineering, Tsinghua University*, Beijing, China.

Research interests

Weathering, Rock microstructure, Neutron scattering, Reactive transport, Mineral reactivity

Professional experience

2021–present **Experimental Geochemist (temporary)**, *Environmental Sciences Division, Oak Ridge National Laboratory*.

2020–2021 **Assistant Research Professor**, *Department of Geosciences, Pennsylvania State University*, University Park, PA.

2018–2020 **Postdoctoral Scholar**, *Department of Geosciences, Pennsylvania State University*, University Park, PA.

Publication

Peer-reviewed journal articles

29. Ruxue Liao, **Xin Gu**, Susan L. Brantley. "Weathering of chlorite from grain to watershed: the role and distribution of oxidation reactions in the subsurface." *Geochimica et Cosmochimica Acta*, 2022, 333, 284-307.

28. **Xin Gu**, Susan L. Brantley. "How particle size influences oxidation of ancient organic matter during weathering of black shale." *ACS Earth and Space Chemistry*, 2022, 6, 1443-1459.

27. **Xin Gu**, Hyojin Kim, Scott Hynek, Aaron Thompson, Susan L. Brantley. "Subsurface particle transport shapes the deep critical zone in a granitoid watershed." *Geochemical Perspectives Letters*, 2021, 19, 13-18

26. Wei Wang, Andrew Nyblade, Gregory Mount, Seulgi Moon, Po Chen, Natalie Accardo, **Xin Gu**, Brandon Forsythe, Susan L. Brantley. "3D seismic anatomy of a watershed reveals climate-topography coupling that drives water flowpaths and bedrock weathering." *Journal of Geophysical Research: Earth Surface*, 2021, 126, e2021JF006281.

25. Lisa Ma, David Oakley, Andrew Nyblade, Seulgi Moon, Natalie Accardo, Wei Wang, **Xin Gu**, Kristen Brubaker, Gregory J. Mount, Brandon Forsythe, Bradley J. Carr, Susan L. Brantley. "Seismic imaging of a shale landscape under compression shows limited influence of topography-induced fracturing." *Geophysical Research Letters*, 48 (17), e2021GL093372

24. Virginia Marcon, Beth Hoagland, **Xin Gu**, Wenjing Liu, Jason Kaye, Roman A. DiBiase, Susan L. Brantley. "How the capacity of bedrock to collect dust and produce soil affects phosphorus bioavailability in the northern Appalachian Mountains of Pennsylvania." *Earth Surface Processes and Landforms*, 2021, 46, 2807-2823.

23. Andrew Shaughnessy, **Xin Gu**, Tao Wen, Susan L. Brantley. "Deciphering the impacts of sulfide oxidation on the CO_2 weathering sink." *Hydrology and Earth System Sciences*, 2021, 25, 3397-3409

22. David Oakley, Brandon Forsythe, **Xin Gu**, Andrew A. Nyblade, Susan L. Brantley. "Seismic ambient noise analyses reveal changing temperature and water signals to 10s of meters depth in the critical zone." *Journal of Geophysical Research: Earth Surface*, 2021, 126, e2020JF005823

21. Larry M. Anovitz, Michael C. Cheshire, Raphael P. Hermann, **Xin Gu**, Julia M. Sheets, Susan L. Brantley, David R. Cole, Eugene S. Ilton, David F. R. Mildner, Cedric Gagnon, Lawrence F. Allard, Kenneth C. Littrell. "Oxidation and associated pore structure modification during experimental alteration of granite." *Geochimica et Cosmochimica Acta*, 2021, 292, 532-556

20. **Xin Gu**, Peter Heaney, Fabio D. A. Aarao Reis, Susan L. Brantley. "Deep abiotic weathering of pyrite." *Science*, 2020, 370 (6515), eabb8092
Highlighted in the weekly newsletter of the Geochemical Society

19. **Xin Gu**, Gary Mavko, Lisa Ma, David Oakley, Natalie Accardo, Bradley J. Carr, Andrew A. Nyblade, Susan L. Brantley. "Seismic refraction tracks porosity generation and possible CO_2 production at depth under a headwater catchment." *Proceedings of the National Academy of Sciences*, 2020, 117 (32), 18991-18997
Highlighted in the weekly newsletter of the Geochemical Society

18. **Xin Gu**, Daniella M. Rempe, William E. Dietrich, A.Joshua West, Teng-Chiu Lin, Lixin Jin, Susan L. Brantley. "Chemical reactions, porosity, and microfracturing in shale during weathering: the effect of erosion rate." *Geochimica et Cosmochimica Acta*, 2020, 269, 63-100

17. Pamela L. Sullivan, Yves Goddéris, Yuning Shi, **Xin Gu**, Jacques Schott, Elizabeth Hasenmuller, Jason Kaye, Christopher Duffy, Lixin Jin, Susan L. Brantley. "Exploring the effect of aspect to inform future earthcasts of climatedriven changes in weathering of shale." *Journal of Geophysical Research: Earth Surface*, 2019, 124, 974-993

16. Susan L Brantley, Tim White, Nicole West, Jennifer Z Williams, Brandon Forsythe, Dan Shapich, Jason Kaye, Henry Lin, Yuning Shi, Margot Kaye, Elizabeth Herndon, Kenneth J Davis, Yuting He, David Eissenstat, Julie Weitzman, Roman DiBiase, Li Li, Warren Reed, Kristen Brubaker, **Xin Gu**. "Susquehanna Shale Hills Critical Zone Observatory: Shale Hills in the Context of Shavers Creek Watershed." *Vadose Zone Journal*, 2018, 17, 1-19

15. **Xin Gu**, David F. R. Mildner. "Determination of porosity in anisotropic, fractal systems by neutron scattering." *Journal of Applied Crystallography*, 2018, 51, 175-184

14. Kim Hyojin, **Xin Gu**, Susan L. Brantley. "Particle fluxes in groundwater change subsurface shale rock chemistry over geologic time." *Earth and Planetary Science Letters*, 2018, 500, 180-191

13. Elizabeth A. Hasenmueller, **Xin Gu**, Julie N. Weitzman, Thomas S. Adams, Gary E. Stinchcomb, David M. Eissenstat, Patrick J. Drohan, Susan L. Brantley, Jason P. Kaye. "Weathering of rock to regolith: The activity of deep roots in bedrock fractures." *Geoderma*, 2017, 300, 11-31

12. Beth Hoagland, Tess A Russo, **Xin Gu**, Lillian Hill, Jason Kaye, Brandon Forsythe, Susan L. Brantley. "Hyporheic zone influences on concentrationdischarge relationships in a headwater sandstone stream." *Water Resources Research*, 2017, 53, 4643-4667

11. **Xin Gu**, David F. R. Mildner, David R. Cole, Gernot G. Rother, Rudy L. Slingerland, Susan L. Brantley. "Quantification of organic porosity and water accessibility in Marcellus shale using neutron scattering." *Energy & Fuels*, 2016, 30, 4438-4449.
Top 25 most cited articles in 2016 published in Energy & Fuels.

10. **Xin Gu**, David F. R. Mildner. "Ultra small-angle neutron scattering with azimuthal asymmetry." *Journal of Applied Crystallography*, 2016, 49, 934-943

9. Pamela L. Sullivan, Scott A. Hynek, **Xin Gu**, Kamini Singha, Timothy White, Nicole West, Hyojin Kim, Brian Clarke, Eric Kirby, Christopher Duffy, Susan L. Brantley. "Oxidative Dissolution under the Channel Leads Geomorphological Evolution at the Shale Hills Catchment." *American Journal of Science*, 2016, 316, 981-1026

8. **Xin Gu**, David R. Cole, Gernot G. Rother, David F. R. Mildner, Susan L. Brantley. "Pores in Marcellus Shale: A neutron scattering and FIB-SEM study." *Energy & Fuels*, 2015, 29, 1295-1308.
Top 25 most cited articles in 2015 published in Energy & Fuels.

7. Victor Balashov, Terry Engelder, **Xin Gu**, Matthew Fantle, Susan L. Brantley. "A model describing flowback chemistry changes with time after Marcellus Shale hydraulic fracturing." *AAPG Bulletin*, 2015, 99, 143-154

6. Timothy M. Byrne, **Xin Gu**, Pin Hou, Fred S Cannon, Nicole R. Brown and Cesar Nieto Delgado. "Quaternary nitrogen activated carbons for removal of perchlorate with electrochemical regeneration." *Carbon*, 2014, 73, 1-12

5. Pin Hou, Fred S. Cannon, Cesar Nieto Delgado, Nicole R. Brown and **Xin Gu**. "Effect of preparation protocol on anchoring quaternary ammonium/epoxide-forming compound into granular activated carbon for perchlorate adsorption: Enhancement by Response Surface Methodology." *Chemical Engineering Journal*, 2013, 223, 309-317.

4. Pin Hou, Fred S. Cannon, Nicole R. Brown, Timothy Byrne, **Xin Gu** and Cesar Nieto Delgado. "Granular activated carbon anchored with quaternary ammonium/epoxide-forming compounds to enhance perchlorate removal from groundwater." *Carbon*, 2013, 53, 197-207.

3. **Xin Gu**, Yu Zhang, Jing Zhang, Min Yang, Hideyuki Tamaki, Yoichi Kamagata and Dong Li. "Isolation of phylogenetically diverse nonylphenol ethoxylate-degrading bacteria and characterization of their corresponding biotransformation pathways." *Chemosphere*, 2010, 3, 216-222.

2. Dong Li, Min Yang, Jianying Hu, Jing Zhang, Ruyin Liu, **Xin Gu**, Yu Zhang and Zhenyu Wang. "Antibiotic-resistance profile in environmental bacteria isolated from penicillin production wastewater treatment plant and the receiving river." *Environmental Microbiology*, 2009, 11, 1506-1517.

1. **Xin Gu**, Yu Zhang, Jing Zhang, Min Yang, Hideyuki Tamaki, and Yoichi Kamagata. "Degradation behaviors of nonylphenol ethoxylates by isolated bacteria using improved isolation method." *Journal of Environmental Sciences*, 2008, 20, 1025-1027.

Funding

- Xin Gu (Principle Investigator) with Susan L. Brantley. "Investigating the role of deep weathering in retention and reaction of chlorinated solvents in a contaminated, fractured bedrock aquifer". United States Geological Survey 104B award from the Pennsylvania Water Resources Research Center (PA-WRRC), $30,000 (2021-2022)

Teaching and mentoring experience

2018, 2021 **Lecturer**, *Pennsylvania State University*, Kinetics of Geochemical Processes.

2016 **Teaching Assistant**, *Pennsylvania State University*, Chemical Processes in Geology.

2015 **Teaching Assistant**, *Pennsylvania State University*, Geology of Oil and Gas.

2014-2016 **Teaching Assistant**, *Pennsylvania State University*, Techniques in Environmental Geochemistry.

2013 **Teaching Assistant**, *Pennsylvania State University*, Environmental Geology.

Students mentored

Ruxue Liao (Visiting PhD student from Lanzhou U, PSU, 2019-2021), Porraket Dechdacho (BSc, PSU, 2020)

Professional/Academic Honors and Awards

2022 Smallest Crack Award in PRF2022

2021 ACS GEOC Early Career Scientist Travel Award

2016 Shell Geosciences Energy Research Facilitation Award (Geosciences at Penn State)

2016 Shell Geosciences Energy Research Facilitation Award (Geosciences at Penn State)

2014 Pittsburgh Association of Petroleum Geologists Named Grant (AAPG Foundation Grants-in-Aid Program)

2014 Chesapeake Energy Scholarship (Geosciences at Penn State)

2007, 2006 Excellence Research Scholarship (Research Center for Eco-Environmental Science, Chinese Academy of Science)

2005 Excellent Student in Academy, Moral and Health (Graduate University of the Chinese Academy of Sciences)

Service to scientific community and outreach

Session and workshop co-convener

- ACS 2022 Fall Meeting session entitled "Multi-scale approaching to understand geochemical dynamic of carbon"
- ACS 2022 Spring Meeting session entitled "Mineral-Water Interactions over Multiple Scales - Connection between Laboratory and Field Scale Observations"
- ACS 2020 Spring Meeting session entitled "Iron Oxides: Their Phase Transformations, Structures, Kinetics, & Applications"
- AGU 2017 Fall Meeting session entitled "Shale Across All Scales" (Union Session)

Invited presentations

- NCNR Seminar, NIST Center for Neutron Research (Aug 2022)
- Goldschmidt 2022 in session "The Role of Fluid-Mineral Interactions During Mineral Alteration, Microstructure Development, Elemental Redistribution and Fractionation" (Jul 2022)
- SSRL/LCLS user meeting 2021 in session "Synchrotron and Neutron Investigations of Deep

subsurface Energy Systems" (Sep 2021)
- ACS 2021 Spring Meeting in session "Fundamental Reactions Driving Macroscopic Geochemical Processes" (Apr 2021)
- AGU 2020 Fall meeting in session "Earth Surface Processes and the Global Carbon Cycle" (Dec 2020)
- Interagency Conference on Research in the Watersheds (ICRW7) in session "Bedrock Flow and Reactions: Implications for Ecohydrology and Watershed Exports" (Nov 2020)
- Geosciences Colloquium, Penn State (Sep 2020)
- Goldschmidt 2020 in session "Long-Term Terrestrial Climate Change, Modern Quantification, and Implications for Extraterrestrial Environments" (Jun 2020)
- Millennium Cafe, Penn State (Feb 2016)
- Pittsburgh Association of Petroleum Geologists April 2015 meeting (Apr 2015)

Reviewer (number of manuscripts)

PNAS (1), Science Advances (1), Nature Communication (3), Geology (1), Earth and Planetary Science Letters (1), Geophysical Research Letters (1), Geochimica et Cosmochimica Acta (6), Environmental Science & Technology (2), Water Resources Research (1), AAPG Bulletin (6), Chemical Geology (4), Earth Surface Dynamics (1), Earth Surface Processes and Landforms (1), Energy & fuels (9), Fuel (2), Geophysics (1), Journal of Geophysical Research - Earth Surface (2), Science of the Total Environment (4), Environmental Engineering Science (3), Review of Scientific Instruments (2), and SPE Journal (2).

Research Skills

Laboratory

- Extensive experience in neutron scattering
- Experience with routine operation and sample preparation for Carbon & Sulfur analyzer, X-ray powder diffraction, ion chromatography, scanning electron microscope, transmission electron microscope, X-ray photoelectron spectroscopy and Raman spectroscopy

Computing

- Modeling and data analysis with Matlab
- Reactive transport modeling with CrunchFlow and PHREEQC

Fieldwork

- Stream water, groundwater, soil and rock sampling; field instrumentation