

Rui Zhang

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Personal Summary

- Self-motivated experimentalist and modeler of fluid-rock and fluid-mineral interactions in geo-chemical/physical porous and particle systems.
- Skilled in small-angle scattering combined with simulation and experimental techniques to solve scientific challenges.

Skills & Knowledge

- Expertise in using **1)** ultra-/small-angle neutron scattering and ultra-/small-/wide-angle X-ray scattering for *in situ* and *ex situ* characterization; **2)** Impulse Excitation (resonant frequency technique) for characterizing elastic and anelastic properties of materials; **3)** Piston cylinder for high-pressure and high-temperature material synthesis; **4)** volumetric/gravimetric adsorption/diffusion, pulse-decay/constant-flow permeability, and uniaxial and triaxial compression measurements.
- Familiar with **1)** all-atom simulation including classic and rare event molecular dynamics simulations through LAMMPS, Plumed, and Materials Studio; **2)** numerous *in situ* and *ex situ* characterization techniques including powder X-ray/neutron diffraction, scanning/transmission electron microscopy, X-ray/neutron tomography, inelastic and quasielastic neutron scattering and neutron spin-echo, atomic pair distribution function analysis, X-ray photoelectron spectroscopy, Fourier transform infrared spectroscopy, electron paramagnetic resonance, cryogenic-/nuclear magnetic resonance, low-pressure N₂/CO₂ adsorption, and mercury intrusion porosimetry.

Education

Energy and Mineral Engineering Ph.D. (07/2015 – 12/2018)

Petroleum Engineering M.S. (08/2013 – 12/2015)

Pennsylvania State University, University Park, Pennsylvania

Petroleum and Natural Gas Engineering M.Eng. (09/2010 – 07/2013)

Petroleum Engineering B.Eng. (09/2006 – 07/2010)

Southwest Petroleum University, Chengdu, Sichuan, China

Research Experience

Associate Research Scientist *will start from 07/2023*

Eyring Materials Center, Arizona State University

- Will manage Xenocs small-angle X-ray scattering instrument, SigRay X-ray absorption spectrometer, and STOE transmission X-ray diffractometer
- Will conduct independent and collaborative research using the instruments

Postdoctoral Research Associate *07/2021 – 07/2023*

Chemical Sciences Division, Oak Ridge National Laboratory (advisor: Larry Anovitz)

- Investigated mineral particle aggregation and compaction
- Understood mechanical properties changes of rock cooking
- Synthesized synthetic rocks with various grain/grain interfaces
- Understanding salt crystallization in rock nanopores (in progress)

Research Associate *05/2019 – 07/2021*

Department of Energy and Mineral Engineering, Pennsylvania State University (advisor: Shimin Liu)

- Investigated size-dependent physical and chemical properties of coal nanoparticles
- Investigated confined fluid (methane, CO₂, and H₂O) storage and transport behaviors
- Investigated shape-dependent nanopore evolution under uniaxial compression

Research Assistant *04/2014 – 12/2018*

Department of Energy and Mineral Engineering, Pennsylvania State University (advisor: Shimin Liu)

- Constructed pore accessibility and pore density models to investigate fluid-rock interactions
- Investigated bio-conversion-induced pore structure alteration in coal
- Investigated pore structure evolution under sorptive and noble gas injection in rocks

Visiting Scholar 09/2017 – 03/2018

Neutron Scattering Division, Oak Ridge National Laboratory (advisor: Lilin He)

- Understood mechanisms of temperature-dependent CO₂ capture in polymer-loaded SBA-15
- Participated in collaboration on ion electrosorption in conductive MOF micropores
- Participated in CG-2 GP-SANS beamline cycle services

Publications

Google Scholar: <https://scholar.google.com/citations?user=nJJ8gfsAAAAJ&hl=en> (citation=1000; h-index=16; i10-index=21)

Journal papers (* corresponding author)

1. Paul A. Bosomworth, **Rui Zhang**, and Lawrence M. Anovitz, “Improved calculation of the shear modulus of rectangular prisms from their resonant frequency overtones” manuscript submitted.
2. Ang Liu, Shimin Liu, **Rui Zhang**, Guijie Sang, Kaiwen Xia “Cyclical water vapor sorption-induced structural alterations of mine roof shale” *International Journal of Coal Geology* in print.
3. Juliane Weber, Vitalii Starchenko, Jan Ilavsky, Lawrence F. Allard, Jitendra Mata, Lisa Debeer-Schmitt, Carolyn Grace Cooke, Kenneth C. Littrell, Lilin He, **Rui Zhang**, Andrew G. Stack, Lawrence M. Anovitz “Grain boundary widening controls siderite (FeCO₃) replacement of limestone (CaCO₃)” *Scientific Reports* 13 (2023): 4581.
4. **Rui Zhang**, Shimin Liu, Long Fan, Tomasz P. Blach, and Guijie Sang, “Unraveling high-pressure gas storage mechanisms in shale nanopores through SANS” *Environmental Science: Nano* 8(9) (2021): 2706-2717.
5. Yu Liu, Shimin Liu, **Rui Zhang**, and Yu Zhang, “The molecular model of Marcellus shale kerogen: Experimental characterization and structure reconstruction” *International Journal of Coal Geology* 246 (2021): 103833.
6. **Rui Zhang** and Shimin Liu “Investigating hierarchical gas confinement in high-rank coal through SANS” Invited manuscript for *Energy & Fuel* 35(16) (2021): 13109–13123.
7. **Rui Zhang**, Shimin Liu, and Siyang Zheng, “Characterization of nano-to-micron sized respirable coal dust: Particle surface alteration and the health impact” *Journal of Hazardous Materials* 413 (2021): 125447.
8. **Rui Zhang**, Shimin Liu, Alfonso San-Miguel, Ralf Schweins, Sylvie Le Floch, and Vittoria Pischedda, “Nanoscale coal deformation and alteration of porosity and pore orientation under uniaxial compression: An *in situ* SANS study” Invited manuscript for a special issue of *Rock Mechanics and Rock Engineering* (2021): 1-16.
9. Yang Wang, Caifang Wu, Yong Qin, Shimin Liu, and **Rui Zhang** “Multi-angle investigation of the fractal characteristics of nanoscale pores in the Lower Cambrian Niutitang shale and their implications for CH₄ adsorption” *Journal of Nanoscience and Nanotechnology* 21(1) (2021): 156-167.
10. Guijie Sang, Shimin Liu, Derek Elsworth, **Rui Zhang**, and Markus Bleuel, “Pore-scale water vapor condensation behaviors in shales: An experimental study” *Transport in Porous Media* 135(3) (2020): 713-734.
11. Lilin He, Luming Yang, Mircea Dinca, **Rui Zhang**, and Jianlin Li “Observation of ion electrosorption in metal-organic framework micropores with *in operando* small-angle neutron scattering” *Angewandte Chemie* 132(24) (2020): 9860-9866.
12. **Rui Zhang**, Shimin Liu, Lilin He, Tomasz P. Blach, and Yi Wang, “Characterizing anisotropic pore structure and its impact on gas storage and transport in coalbed methane and shale gas reservoirs” *Energy & Fuels* 34(3) (2020): 3161-3172.

13. Shimin Liu and **Rui Zhang**^{*}, “Anisotropic pore structure of shale and gas injection-induced nanopore alteration: A small-angle neutron scattering study” *International Journal of Coal Geology* 219 (2020): 103384.
14. Yang Wang, Yanming Zhu, **Rui Zhang**^{*}, Lawrence M. Anovitz, Markus Bleuel, Shimin Liu, and Shangbin Chen, “SANS coupled with fluid invasion approaches for characterization of overall nanopore structure and mesopore connectivity of organic-rich marine shales in China” *International Journal of Coal Geology* 217 (2020): 103343.
15. **Rui Zhang**, Xiaoxing Wang, Shimin Liu, Lilin He, Chunshan Song, Xiao Jiang, and Tomasz P. Blach, “Discovering inherent characteristics of polyethylenimine-functionalized porous materials for CO₂ capture” *ACS Applied Materials & Interfaces* 11(40) (2019): 36515-36524.
16. Yang Wang, Yong Qin, Liu Yang, Shimin Liu, Derek Elsworth, and **Rui Zhang**. “Organic geochemical and petrographic characteristics of the coal measure source rocks of Pinghu Formation in the Xihu Sag of the East China Sea Shelf Basin: Implications for coal measure gas potential” *Acta Geologica Sinica - English Edition* (2019).
17. Shimin Liu, **Rui Zhang**^{*}, Zuleima Karpyn, Hongkyu Yoon, and Thomas Dewers, “Investigation of accessible pore structure evolution under pressurization and adsorption for coal and shale using small-angle neutron scattering” *Energy & Fuel* 33 (2019): 837-847.
18. Hao Xu, Wen Zhou, **Rui Zhang**, Shimin Liu, and Qiumei Zhou, “Characterizations of pore, mineral and petrographic properties of marine shale using multiple techniques and their implications on gas storage capability for Sichuan Longmaxi gas shale field in China” *Fuel* 241 (2019): 360-371.
19. Yang Wang, Yong Qin, **Rui Zhang**^{*}, Lilin He, Lawrence M. Anovitz, Markus Bleuel, David F. R. Mildner, Shimin Liu, and Yanming Zhu, “Evaluation of nanoscale accessible pore structure for improved prediction of gas production potential in Chinese marine shales” *Energy & Fuel* 32 (2018): 12447-12461.
20. Guijie Sang, Shimin Liu, **Rui Zhang**, Derek Elsworth, and Lilin He, “Nanopore characterization of mine shales by SANS, nitrogen adsorption, and mercury intrusion: Impact on water adsorption/retention behavior” *International Journal of Coal Geology* 200 (2018): 173-185.
21. Yang Wang, Caifang Wu, Yanming Zhu, Shangbin Chen, Shimin Liu, and **Rui Zhang**, “Morphology and fractal characterization of multiscale pore structures for organic-rich lacustrine shale reservoirs” *Fractals* 26(2) (2018): 1840013.
22. **Rui Zhang**, Shimin Liu, and Yang Wang, “Fractal evolution under in-situ pressure and sorption conditions for coal and shale” *Scientific Reports* 7 (2017): 8971.
23. **Rui Zhang**, Shimin Liu, Jitendra Bahadur, Derek Elsworth, Yi Wang, Guanglong Hu, and Yanna Liang, “Changes in pore structure of coal caused by coal-to-gas bioconversion” *Scientific Reports* 7 (2017): 3840.
24. **Rui Zhang** and Shimin Liu, “Experimental and theoretical characterization of methane and CO₂ sorption hysteresis in coals based on Langmuir desorption” *International Journal of Coal Geology* 171 (2017): 49-60.
25. Yang Wang, Yanming Zhu, Shimin Liu, Shangbin Chen, and **Rui Zhang**, “Comparative study of nanoscale pore structure of Lower Paleozoic marine shales in the Middle-Upper Yangtze area, China: Implications for gas production potential” *Geological Journal* (2017): 1-14.
26. Yang Wang, Yanming Zhu, Shimin Liu, and **Rui Zhang**, “Pore characterization and its impact on methane adsorption capacity for organic-rich marine shales” *Fuel* 181 (2016): 227-237.
27. Yang Wang, Yanming Zhu, Shimin Liu, and **Rui Zhang**, “Methane adsorption measurements and modeling for organic-rich marine shale samples” *Fuel* 172 (2016): 301-309.
28. **Rui Zhang**, Shimin Liu, Jitendra Bahadur, Derek Elsworth, Yuri Melnichenko, Lilin He, and Yi Wang, “Estimation and modeling of coal pore accessibility using small-angle neutron scattering” *Fuel* 161 (2015): 323-332.

Conference papers

29. **Rui Zhang** and Shimin Liu, “Nanoscale coal deformation and its geomechanics effect on pore structure evolution under hydrostatic and uniaxial compression conditions” *the 53rd US Rock Mechanics/Geomechanics Symposium*. American Rock Mechanics Association (2019).
30. Sang Guijie, Shimin Liu, **Rui Zhang**, and Derek Elsworth, “Pore characterization of mine shales by low-pressure nitrogen adsorption and mercury intrusion porosimetry: Implication on water retention behavior of shales” *the 52nd US Rock Mechanics/Geomechanics Symposium*. American Rock Mechanics Association (2018).

Conference Presentations

1. “Effect of Dry and Wet Annealing on the Mechanical Properties of Limestones” Poster presentation at *AGU Fall Meeting 2022*, Chicago, IL. December 16, 2022.
2. “Effect of Dry Annealing on the Mechanical Properties of Limestones” Poster presentation at *Goldschmidt 2022*, Honolulu, HI. July 11, 2022.
3. “Investigating Effects of Salt Concentration and External Force on Compaction of Mineral Nanoparticles” Oral presentation at *ACS Spring 2022*, March 21, 2022 (online).
4. “Investigation of Kerogen Structures through Simulation and Scattering Approaches” Oral presentation at *the 10th American Conference on Neutron Scattering*, July 13-16, 2020 (online).
5. “Alteration of Shale Anisotropic Pores under Uniaxial Compression Condition: An Investigation Using Small-Angle Neutron Scattering” Poster presentation at *AGU Fall Meeting 2019*, San Francisco, CA. December 11, 2019.
6. “Anisotropic Pore Structure of Marcellus Shale under Uniaxial Compression: A Small-Angle Neutron Scattering Study” Oral presentation at *2019 AAPG Eastern Section Annual Meeting*, Columbus, OH. October 14, 2019.
7. “Characterization of Anisotropic Nanopore Structure of Organic-rich Marine Shales in China: A SANS Study” Oral presentation at *2019 ACA Annual Meeting*, Covington, KY. July 21, 2019.
8. “Nanoscale Coal Deformation and Its Geomechanics Effect on Pore Structure Evolution Under Hydrostatic and Uniaxial Compression Conditions” Oral presentation at *the 53rd US Rock Mechanics/Geomechanics Symposium*. American Rock Mechanics Association, New York City, NY. June 26, 2019.
9. “Gas Densification and Adsorption in Rock Nanopores” Oral presentation at *International Small-Angle Scattering Conference*, Treasure City, MI. October 11, 2018.
10. “Investigation of Shale Matrix Heterogeneity, Anisotropy, and Strain Using X-Ray and In-Situ Neutron Diffraction” Poster presentation at *Goldschmidt 2018*, Boston, MA. August 16, 2018.
11. “Observation of Anisotropic Nanoscale Accessible Pore Structure for Anthracite and Shale Using Small-Angle Neutron Scattering” Oral presentation at *the 9th American Conference on Neutron Scattering*, College Park, MD. June 25, 2018.
12. “Nanoscale Accessible Pore Structure Characterization for Improved Prediction of Gas Production Potential in Organic-Rich Shales” Poster presentation at *Marcellus Shale Coalition Meeting*, University Park, PA. April 11, 2018.

Professional Activities

Co-organizer of the *Frontiers in Multi-scale and Multi-approach Characterization of Fine-grained Geomaterials* session in *AGU Fall 2023*. San Francisco, CA. December 11-15, 2023.

Co-editor of the *Safe Mining and Disaster Prevention of Deep Coal Resources* research topic in *Frontiers in Earth Science* journal in 2023.

Invited talk in *Reactivity at the Mineral-Water Interface: Validation through Modeling and Experiments at the Pore Scale* session in *ACS Fall 2023*. August 13-17, 2023.

Editorial board member on the “Geo-Energy” section of *Energies* journal starting from 2023.

Co-organizer of the *Multi-scale Geochemical Approaches in CO₂ Capture, Conversion, and Sequestration* session in *ACS Fall 2022*. Chicago, IL. August 21-25, 2022.

Invited talk in *New Chemistry Driven by Extremes Workshop in Virtual Joint Nanoscience and Neutron Scattering User Meeting*, online. August 4, 2021.

Invited talk and discussion in the *soft matter* breakout session of *New Science Opportunities with Small and Wide-Angle Neutron Diffractometer/Spectrometer at Second Target Station at SNS/ORNL Workshop*, online. February 26, 2021. Contributed to selecting CENTAUR, a small-/wide-angle scattering instrument at the Second Target Station at SNS/ORNL.

Co-chair in the *Morphological Characterization of Porous Materials* session at the *2019 ACA Annual Meeting*, Covington, KY. July 21, 2019.

Co-chair in the *Coal, CBM, and Gas Hydrate Geomechanics* session in the *53rd US Rock Mechanics/Geomechanics Symposium*. American Rock Mechanics Association, New York City, NY. June 24, 2019.

Peer reviewer (about 50 papers) of journals including *Chemical Engineering Journal*, *Environmental Science & Technology*, *International Journal of Coal Geology*, *Scientific Reports*, *Fuel*, *Energy & Fuels*, *Journal of Petroleum Science and Engineering*, *ACS Omega*, *Minerals*, *Energies*, *Water*, *Geofluids*, *Review of Scientific Instruments*, etc.

Peer reviewer (about 10 abstracts and 5 papers) of conference abstracts and papers of the *53rd US Rock Mechanics/Geomechanics Symposium*. American Rock Mechanics Association.

Peer reviewer of beamtime proposals of *CG-2 GP-SANS at HFIR/ORNL* in 2021.

Awards & Honors

The Charles B. Darrow Award, Pennsylvania State University, 2017 and 2018

Frank J. Vastola and Ruth J. St. Clair Vastola Graduate Scholarship, Pennsylvania State University, 2018