

Jue Liu

Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831

Email: liuj1@ornl.gov; Phone: 631-488-7719

Research interests

Crystallography, neutron and X-ray diffraction, pair distribution function, rechargeable batteries, solid state chemistry, nano-catalysis

Education

Ph.D. Stony Brook University (2010-2015)
Chemistry
Advisors: Prof. Peter Khalifah and Dr. Xiao-Qing Yang

B.S. University of Science and Technology of China (USTC) (2006-2010)
Materials Science and Engineering

Research Activities and Employment

2018-	<i>Instrument scientist</i>	Neutron Scattering Division, Oak Ridge National Lab
2016-2018	<i>Post-doc</i>	Neutron Scattering Division, Oak Ridge National Lab Supervisor: Dr. Katharine Page
2010-2015	<i>Research assistant</i> <i>Research assistant</i>	Department of Chemistry, Stony Brook University Chemistry Division, Brookhaven National Lab

Publication (> 70 publications, > 4000 citations; * corresponding author, #equal contribution)

1. **Liu, J.***; Du, Z.; Wu, X.; Geng, L.; Song, B.; Chien, P.-H.; Everette, S. M., Anion redox induced anomalous structural transition in Ni-rich cathode. In revision, *Energy & Environmental Science*
2. Wu, X.; Song, B.; Chien, P.-H.; Everett, S. M.; Zhao, K.; **Liu, J.***; Du, Z.*, Structural Evolution and Transition Dynamics in Lithium Ion Battery under Fast Charging: An *Operando* Neutron Diffraction Investigation. *Adv. Sci.* 2021, 2102318.
3. Chien, P.-H.; Wu, X.; Song, B.; Yang, Z.; Waters, C. K.; Everett, M. S.; Lin, F.; Du, Z.*; **Liu, J.***, New Insights into Structural Evolution of LiNiO₂ Revealed by *Operando* Neutron Diffraction. *Batteries & Supercaps*, 2021. (**front cover**)
4. Patel, S. V.; Banerjee, S.; Liu, H.; Wang, P.; Chien, P.-H.; Feng, X.; **Liu, J.**; Ong, S. P.; Hu, Y.-Y., Tunable Lithium-Ion Transport in Mixed-Halide Argyrodites Li_{6-x}PS_{5-x}ClBr_x: An Unusual Compositional Space. *Chem. Mater.* 2021, 33, 1435-1443.
5. Hu, E.; Li, Q.; Wang, X.; Meng, F.; **Liu, J.**; Zhang, J.-N.; Page, K.; Xu, W.; Gu, L.; Xiao, R.; Li, H.; Huang, X.; Chen, L.; Yang, W.; Yu, X.; Yang, X.-Q., Oxygen-redox reactions in LiCoO₂ cathode without O-O bonding during charge-discharge. *Joule* 2021, 5, 720-736.
6. Kong, J.; **Liu, J.**; Marlton, F.; Jørgensen, M. R. V.; Pramanick, A., A Structural Study of 0.06LiNbO_{3-0.94}K_{0.5}Na_{0.5}NbO₃ from Neutron Total Scattering Analysis. *Crystals* 2021, 11, 395.

7. Kong, J.; **Liu, J.**; Marlton, F.; Jørgensen, M. R. V.; Pramanick, A., Local structural mechanism for phase transition and ferroelectric polarization in the mixed oxide. *Phys. Rev. B* 2021, 103, 184104.
8. Kim, S. Y.; Kaup, K.; Park, K.-H.; Assoud, A.; Zhou, L.; **Liu, J.**; Wu, X.; Nazar, L. F., Lithium Ytterbium-Based Halide Solid Electrolytes for High Voltage All-Solid-State Batteries. *ACS Materials Letters* 2021, 3, 930-938.
9. Zheng, X.; Xu, Z.; Li, S.; Zhang, Y.; Zhang, J.; Kuai, C.; Tao, L.; Rahman, M. M.; Zhang, Y.; Lee, S.-J.; Sun, C.-J.; Li, L.; Hu, W.; Nordlund, D.; **Liu, J.**; Liu, Y.; Lin, F., Reversible Mn/Cr dual redox in cation-disordered Li-excess cathode materials for stable lithium ion batteries. *Acta Mater.* 2021, 212, 116935.
10. Rahman, M. M.; McGuigan, S.; Li, S.; Gao, L.; Hou, D.; Yang, Z.; Xu, Z.; Lee, S.-J.; Sun, C.-J.; **Liu, J.**; Huang, X.; Xiao, X.; Chu, Y.; Sainio, S.; Nordlund, D.; Kong, X.; Liu, Y.; Lin, F., Chemical modulation of local transition metal environment enables reversible oxygen redox in Mn-based layered cathodes. *ACS Energy Letters* 2021, 6, 2882-2890.
11. Liang, G.; Peterson, V. K.; Wu, Z.; Zhang, S.; Hao, J.; Lu, C.-Z.; Chuang, C.-H.; Lee, J.-F.; **Liu, J.**; Leniec, G.; Kaczmarek, S. M.; D'Angelo, A. M.; Johannessen, B.; Thomsen, L.; Pang, W. K.; Guo, Z., Crystallographic-Site-Specific Structural Engineering Enables Extraordinary Electrochemical Performance of High-Voltage LiNi_{0.5}Mn_{1.5}O₄ Spinel Cathodes for Lithium-Ion Batteries. *Adv. Mater.* 2101413.
12. Self, E. C.; Chien, P.-H.; O'Donnell, L. F.; Morales, D.; **Liu, J.**; Brahmabhatt, T.; Greenbaum, S.; Nanda, J., Investigation of glass-ceramic lithium thiophosphate solid electrolytes using NMR and neutron scattering. *Materials Today Physics* 2021, 21, 100478.
13. Wang, C.; Liang, J.; Luo, J.; **Liu, J.**; Li, X.; Zhao, F.; Li, R.; Huang, H.; Zhao, S.; Zhang, L.; Wang, J.; Sun, X., A universal wet-chemistry synthesis of solid-state halide electrolytes for all-solid-state lithium-metal batteries. *Sci. Adv.* 2021, 7, eabh1896.
14. Kaup, K.; Bishop K.; Assoud, A.; **Liu, J.**; Nazar, L.F., Fast Ion-Conducting Thioboracite with a Perovskite Topology and Argyrodite-like Lithium Substructure. *J. Am. Chem. Soc.* 2021, 143, 6952-6961.
15. Luo, S.; Li, M.; Fung, V.; Sumpter, B.G.; **Liu, J.***; Wu, Z.*; Page, K*., New insights into the bulk and surface defect structures of ceria nanocrystals from neutron scattering study. *Chem. Mater.* 2021, 33, 3959-3970.
16. Kaup, K.; Assoud, A.; **Liu, J.**; Nazar, L., Fast Li-Ion Conductivity in Superadamantanoid Lithium Thioborate Halides. *Angew. Chem. Int. Ed.* 2021, 60, 6975-6980.
17. Liu, Z.; Ma, S.; **Liu, J.**; Xiong, S.; Ma, Y.; Chen, H., High Ionic Conductivity Achieved in Li₃Y(Br₃Cl₃) Mixed Halide Solid Electrolyte via Promoted Diffusion Pathways and Enhanced Grain Boundary. *ACS Energy Letters* 2021, 6, 298-304.
18. Parejiya, A.; Essehli, R.; Amin, R.; **Liu, J.**; Muralidharan, N.; Meyer, H. M.; Wood, D. L.; Belharouak, I., Na_{1+x}Mn_{x/2}Zr_{2-x/2}(PO₄)₃ as a Li⁺ and Na⁺ Super Ion Conductor for Solid-State Batteries. *ACS Energy Letters* 2021, 429-436.
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20. Wang, F.; Evans, H. A.; Kim, K.; Yin, L.; Li, Y.; Tsai, P.-C.; **Liu, J.**; Lapidus, S. H.; Brown, C. M.; Siegel, D. J.; Y. Chiang, "Dynamics of Hydroxyl Anions Promotes Lithium Ion Conduction in Antiperovskite Li₂OHCl." *Chem. Mater.* 2020, 32, 8481-8491.
21. Wang, J.; Wang, X.; Liu, B.; Lu, H.; Chu, G.; **Liu, J.**; Guo, Y.-G.; Yu, X.; Luo, F.; Ren, Y.; Chen, L.; Li, H., Size effect on the growth and pulverization behavior of Si nanodomains in SiO anode. *Nano Energy* 2020, 78, 105101.

22. Wu, X.; Bai, Y.; Li, Z.; **Liu, J.**; Zhao, K.; Du, Z., “Effects of charging rates on LiNi_{0.6}Mn_{0.2}Co_{0.2}O₂ (NMC622)/graphite Li-ion cells.” *Journal of Energy Chemistry*, 56, 121-126. (2020).
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26. Li, C.; Zhang, Y.; **Liu, J.**; Graetsch, H. A., “Long-Range and Local Structure of Sr_xBa_{1-x}Nb₂O₆ (x= 0.33 and 0.67) across the Ferroelectric–Relaxor Transition.” *Chem. Mater.*, 32, 1844-1853. (2020)
27. Ji, H.; Wu, J.; Cai, Z.; **Liu, J.**; Kwon, D.-H.; Kim, H.; Urban, A.; Papp, J. K.; Foley, E.; Tian, Y., Ultrahigh power and energy density in partially ordered lithium-ion cathode materials. *Nat. Energy*, 5, 213-221.(2020)
28. Muralidharan, N.; Essehli, R.; Hermann, R. P.; Amin, R.; Jafta, C.; Zhang, J.; **Liu, J.**; Du, Z.; Meyer III, H. M.; Self, E., “Lithium Iron Aluminum Nickelate, LiNi_xFe_yAl_zO₂—New Sustainable Cathodes for Next-Generation Cobalt-Free Li-Ion Batteries.” *Adv. Mater.*, 32, 2002960. (2020)
29. Zhao, E., Zhang, M., Wang, X., Hu, E., **Liu, J.***, Yu, X.*, Olguin, M., Wynn, T.A., Meng, Y.S.*, Page, K., Wang, F., “Local structure adaptability through multi cations for oxygen redox accommodation in Li-Rich layered oxides.” *Energy Storage Materials*, 24, 384-393. (2020) [[doi](#)]
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31. **Liu, J.***, Wang, X., Borkiewicz, O.J., Hu, E., Xiao, R.J., Chen, L., Page, K.*, “Unified View of the Local Cation-Ordered State in Inverse Spinel Oxides.” *Inorg. Chem.*, 58, 14389-14402. (2019) [[doi](#)]
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33. Luo, S., **Liu, J.**, Wu, Z. “Interaction of SO₂ with ZnO Nanoshapes: Impact of Surface Polarity.” *J. Phys. Chem. C* 123, 11772-11780. (2019) [[doi](#)]
34. Song, B., Tang, M., Hu, E., Borkiewicz, O.J., Wiaderek, K.M., Zhang, Y., Phillip, N.D., Liu, X., Shadike, Z., Li, C., Song, L., **Liu, J.*** et al. “Understanding the Low Voltage Hysteresis of Anionic Redox in Na₂Mn₃O₇.” *Chem. Mater.*, 31, 3756-3765. (2019) [[doi](#)]
35. Yang, L., Li, X., **Liu, J.**, Xiong, S., Ma, X., Liu, P., Bai, J., Xu, W., Tang, Y., Hu, Y.Y., Liu, M., 2019. “Lithium-Doping Stabilized High-Performance P2–Na_{0.66}Li_{0.18}Fe_{0.12}Mn_{0.7}O₂ Cathode for Sodium Ion Batteries.” *J. Am. Chem. Soc.*, 141, 6680-6689. (2019) [[doi](#)]
36. Zhao, E., Li, Q., Meng, F., **Liu, J.**, Wang, J., He, L., Jiang, Z., Zhang, Q., Yu, X., Gu, L. Yang, W., “Stabilizing the Oxygen Lattice and Reversible Oxygen Redox Chemistry through Structural Dimensionality in Lithium-Rich Cathode Oxides.” *Angewandte Chemie International Edition*, 58, 4323-4327. (2019)
37. Zhang, P., **Liu, J.**, Page, K. and Navrotsky, A., “Calorimetric study of the thermodynamic properties of Mn₅O₈.” *Journal of the American Ceramic Society*, 102, 1394-1401.(2019) [[doi](#)]

38. Song, B., Hu, E., **Liu, J.***, Zhang, Y., Yang, X.Q., Nanda, J., Huq, A.*, Page, K.* “A novel P3-type $\text{Na}_{2/3}\text{Mg}_{1/3}\text{Mn}_{2/3}\text{O}_2$ as high capacity sodium-ion cathode using reversible oxygen redox.” *J. Mater. Chem. A*, 7, 1491-1498. (2019) [[doi](#)] (**Back Cover**)
39. Song, B., Veith, G.M., Park, J., Yoon, M., Whitfield, P.S., Kirkham, M.J., **Liu, J.**, Huq, A. “Metastable $\text{Li}_{1+\delta}\text{Mn}_2\text{O}_4$ ($0 \leq \delta \leq 1$) Spinel Phases Revealed by in Operando Neutron Diffraction and First-Principles Calculations. *Chem. Mater.*, 31, 124-134. (2018) [[doi](#)]
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Patent

1. Khalifah, P. G.; **Liu, J.**; “Cubic Ionic Conductor Ceramics for Alkali Ion Batteries” *US Patent* 20,130,316,250. (2013) [[link](#)]

Funding

LDRD-2021, ORNL, PI, “Operando neutron total scattering for battery research” (725 K for two years), awarded.

LDRD-2021, ORNL, Co-PI, “Automatic Structure Refinement Platform (ASRP) for neutron diffraction” (PI, Wenduo Zhou, 444 K for two years), awarded.

DOE-FOA, Co-PI, “Integrated Computational and Experimental Investigation on Lithium REE Halide Solid Superionic Conductors” (PI, Yifei Mo, University of Maryland), pending.

Professional Memberships, services and outreach activities

- Members of American Crystallography Association (ACA), Neutron Scattering Society of America (NSSA), American Chemical Society (ACS), Electrochemical Society (ECS), Materials Research Society (MRS) and American Ceramic Society (ACerS).
- Served as Referees for: Nature Materials, Nature Communications, Journal of the American Chemical Society, Journal of Applied Crystallography, ACS Energy Letters, Energy & Environmental Science, Chemistry of Materials, Inorganic Chemistry, ACS Applied Materials & Interface, Journal of Industry chemistry, Journal of the Electrochemical Society etc.
- Served as Judge for the Pauling poster prize, American Crystallography Association

- Co-organizer, “ENFL electrolyte and interfaces symposium”, ACS 2022 spring meeting. (2022)
- Co-organizer, “Materials Synthesis Science and Opportunities Aided by in-situ Scattering Tools”, 2021 Joint nanoscience and neutron scattering user meeting, ORNL, August 2021.
- Co-organizer and Instructor, “Modern Methods in Rietveld Refinement and Structural Analysis”, a 5-day national summer school on the structural analysis of diffraction data from laboratory, synchrotron, and time-of-flight neutron sources (2017).

Presentation and workshop

1. CNMS (ORNL) seminar 2021, virtual, Oct 2021 (**invited talk**)
“Neutron total scattering and its application in studying energy materials”
2. ACA meeting 2021, virtual, Aug 2021 (**invited talk**)
“*In situ* neutron diffraction for rechargeable battery research”
3. MRS fall meeting 2020, virtual, Nov 2020 (**invited tutorial talk**)
“*In situ* neutron diffraction for rechargeable battery research”
4. ICACC 2020 Daytona Beach, FL, Jan 2020 (**invited talk**)
“Reversible Anionic Redox in New Layered Na-Ion Cathodes”
5. 2019 ECS fall meeting, Atlanta, GA, Oct 2019
“Understanding the Reversible Anionic Redox in New Layered Na-Ion Cathodes”
6. Joint ORNL-Georgia Tech energy storage workshop, GA, May 2019
“The application of neutron scattering in studying battery materials”
7. Third US school on Total Scattering Analysis, Oak Ridge, TN, Oct 2019
Instructor, Small box modeling using pair distribution function
8. Second US school on Total Scattering Analysis, Oak Ridge, TN, Aug 2018
Instructor, Small box modeling using pair distribution function
9. Modern Methods in Rietveld Refinement for Structural Analysis, Oak Ridge, TN, June 2017
Instructor, neutron diffraction and pair distribution function section.
10. First US school on Total Scattering Analysis, Oak Ridge, TN, May 2017 (dinner talk)
“Quantitative analysis of the morphology of faceted anatase TiO₂ nanocrystals using total scattering”
11. 2016 American Conference on Neutron Scattering, Long Beach, CA, July 2016
“Understanding the rapid reversible phase transformation between nanophase bixbyite (Mn₂O₃) and hausmannite (Mn₃O₄) triggered by surface water using neutron total scattering”
12. 2016 Solid State Chemistry Gordon Conference, New London, NH, July 2016 (poster)
“Neutron PDF investigation of nanoscale Ni/Mn ordering in high voltage LiNi_{0.5}Mn_{1.5}O₄”
13. 2016 China International Batter Fair, Shenzhen, May 2016 (**invited talk**)

“Combined synchrotron X-ray and neutron scattering study of cathode materials for rechargeable batteries”

14. RMCprofile workshop, Oak Ridge, TN, February 2016 (**invited talk**)
“Quantifying stacking faults in honeycomb-ordered layered oxides”
15. 2014 ACS Fall Meeting, San Francisco, CA, Aug 2014 (**invited talk**)
“Monitoring mobile ions: X-ray and neutron diffraction studies of emerging battery materials”
16. 2014 ACS Fall Meeting, San Francisco, CA, Aug 2014
“Synthesis and structure study of two new lithium nitridophosphates”
17. 2014 Solid State Chemistry Gordon Conference, New London, NH, July 2014 (poster)
“Li⁺/Na⁺ mobility and ion exchange in CUBICONS: *in situ* neutron diffraction studies”
18. 2013 MRS Fall Meeting, Boston, MA, USA, Dec 2013
“Novel Cathode Framework for Na-ion Batteries”

Honors

President’s award, Stony Brook University, 2016

Best tutorial award, Materials Research Society, 2020

Student and postdoc supervised

Shantonio Brich, GEM student, University of Michigan (success story link:

<https://orise.orau.gov/ornl/experiences/graduate/birch.html>)

Bohang Song, postdoc (co-advised with Ashfia Huq, success story link:

<https://www.ornl.gov/file/postdoctoral-opportunities-fact-sheet/display>), now team leader at BASF, OH

Yiman Zhang, postdoc (partially co-advised with Jagjit Nanda), now senior engineer at Honda North America, CA

Po-Hsiu Chien, now scientist at A123, MA

Xianyang Wu, current visiting student from University of Purdue