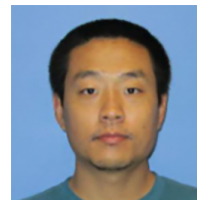# Yuanpeng Zhang, PhD

Email: zhangy3@ornl.gov

Mobile: +1(865)335-4818

ORCID: 0000-0003-4224-3361   Website: https://iris2020.net/

Address: SNS, Oak Ridge National Laboratory, 1 Bethel Valley Rd, Oak Ridge, TN 37830, US

Summary

I love physics, for its beauty of explaining not only the world, but also our life. I love programming, not only for the convenience coming with it, but also for exploring the otherwise untouchable world without it.

I am interested in looking at local structure (both nucleus and magnetic) of various materials through combined experimental and theoretical approaches. This involves the application of experimental techniques (including neutron/X-ray total scattering, X-ray absorption spectroscopy, etc.) and theoretical simulation (molecular dynamics simulation, density functional theory calculation, etc.) to understand materials system in a comprehensive way.

Meanwhile, I have been actively contributing to software development for total scattering data reduction and analysis. This involves the development and maintenance of ADDIE and Mantid for reducing neutron total scattering data, ADDIE on cloud for scattering data analysis and RMCProfile for structure modeling based on supercell approach and reverse Monte Carlo algorithm.

Education

- **Beihang University** — BEIJING, P. R. CHINA
  Bachelor degree in Physics and Nuclear Energy Engineering — *2008 – 2012*

- **Queen Mary, University of London** — LONDON, UNITED KINGDOM
  PhD degree in Condensed Matter and Materials Physics — *2012 – 2016*
    PhD Thesis: Local structure characterization of amorphous and nanoscale systems using X-ray Absorption Spectroscopy (XAS)

Employment

- **Oak Ridge National Laboratory** — OAK RIDGE, UNITED STATES
  Postdoc Research Assistant — *2017 – 2019*

- **National Institute of Standards and Technology** — Maryland, United States
  &
  Oak Ridge National Laboratory — OAK RIDGE, UNITED STATES
  Visiting Scientist — *2019 – 2020*

- **Oak Ridge National Laboratory** — OAK RIDGE, UNITED STATES
  Neutron Scattering Scientist — *2020 – Now*

Selected Publications

- H. Liu, X. Shi, Y. Yao, H. Luo, Q. Li, H. Huang, H. Qi, **Y. Zhang**, Y. Ren, S. D Kelly, K. Roleder, J. C. Neuefeind, L. Chen, X. Xing, and J. Chen, Emergence of high piezoelectricity from competing local polar order-disorder in relaxor ferroelectrics, *Nat. Commun.*, 2023, **145**, 6194-6202.

- Z. Sun, J. Zhang, H. Luo, Y. Yao, N. Wang, L. Chen, T. Li, C. Hu, H. Qi, S. Deng, L. C. Gallington, **Y. Zhang**, J. C Neuefeind, H. Liu, and J. Chen, Superior Capacitive Energy-Storage Performance in Pb-Free Relaxors with a Simple Chemical Composition, *J. Am. Chem. Soc.*, 2023, **145**, 6194-6202.

- **Y. P. Zhang***, J. Liu, and M. G. Tucker, Lorentz factor for time-of-flight neutron Bragg and total scattering, *Acta Cryst.*, 2023, **A79**, 20-24.

- X. Wang, B. L. Musico, C. Kons, P. C. Metz, V. Keppens, D. A. Gilbert, **Y. P. Zhang**, and K. Page, Local cation order and ferrimagnetism in compositionally complex spinel ferrites, *APL. Mater.*, 2022, **10**, 121102.

- Q. Zhang*, **Y. Zhang***, M. Matsuda, V. O. Garlea, J. Yan, M. A. McGuire, D. A. Tennant and S. Okamoto, https://doi.org/10.1021/jacs.2c05665, *J. Am. Chem. Soc.*, 2022, **144**, 14339-14350.

- F. P. Marlton, S. Nayak, S. Venkateshwarlu, N. H. Chan, J. Kong, **Y. Zhang**, M. G. Tucker, M. R. V. Jorgensen and A. Pramanick, https://doi.org/10.1021/acs.chemmater.1c03066, *Chem. Mater.*, 2021, **32**, 8844–8853.

- X. Wang, B. Jiang, **Y. P. Zhang**, K. Young-II and K. Page, https://doi.org/10.1021/acs.inorgchem.1c01594, *Inorg. Chem.*, 2021, **60**, 14190–14201.

- J. Marcia, **Y. Zhang**, X. Zhao, H. Xu, A. Mesbah, E. T. Nienhuis, S. Szenknect, J. C. Neuefeind, J. Lin, L. Qi, A. A. Migdisov, R. C. Ewing, N. Dacheux , J. S. McCloy and X. Guo, Thermodynamic non-ideality and disorder heterogeneity in actinide silicate solid solutions, *NPJ Mater. Degrad.*, 2021, **5**, 24.

- S. Roy, S. Sharma, W. V. Karunaratne, F. Wu, R. Gakhar, D. S. Maltsev, P. Halstenberg, M. Abeykoon, S. K. Gill, **Y. Zhang**, S. M. Mahurin, S. Dai, V. S. Bryantsev, C. J. Margulis and A. S. Ivanov. X-ray Scattering Reveals Ion Clustering of Dilute Chromium Species in Molten Chloride Medium, *Chem. Sci.*, 2021, **12**, 8026–8035.

- J. Peng, M. Y. Ou, H. C. Yi, X. P. Sun, **Y. P. Zhang**, *et al.*, Defect-free-induced Na+ disordering in electrode materials, *Energy Environ. Sci.*, 2021, **14**, 3130–3140.

- B. Jiang, C. A. Bridges, R. R. Unocic, K. C. Pitike, V. R. Cooper, **Y. P. Zhang**, D. Y. Lin and K. Page, Probing the Local Site Disorder and Distortion in Pyrochlore High-Entropy Oxides, *J. Am. Chem. Soc.*, 2021, **143** (11), 4193–4204.

- F. P. Marlton, Z. M. Zhao, **Y. P. Zhang**, T. E. Proffen, C. D. Ling and B. J. Kennedy, Lattice Disorder and Oxygen Migration Pathways in Pyrochlore and Defect-Fluorite Oxides, *Chem. Mater.*, 2021, **33** (4), 1407–1415.

- **Y. Zhang**, M. Eremenko, V. Krayzman, M. G. Tucker and I. Levin, New capabilities for enhancement of RMCProfile: instrumental profiles with arbitrary peak shapes for structural refinements using the reverse Monte Carlo method, *J. Appl. Crystallogr.*, 2020, **53**, 1509–1518.

- C. Li, **Y. P. Zhang**, J. Liu and H. A. Graetsch. Long-Range and Local Structure of SrxBa1–xNb2O6 (x = 0.33 and 0.67) across the Ferroelectric–Relaxor Transition, *Chem. Mater.*, 2020, **32** (5), 1844–1853.

- Z. Deng, M. Y. Ou, J. Wan, S. Li, Y. Y. Li, **Y. P. Zhang**, *et al.*, Local Structural Changes and Inductive Effects on Ion Conduction in Antiperovskite Solid Electrolytes, *Chem. Mater.*, 2020, **32** (20), 8827–8835.

- **Y. P. Zhang***, M. McDonnell, W. Liu and M. G. Tucker*. Reverse Monte Carlo modeling for low-dimensional systems, *J. Appl. Cryst.*, 2019, **52**, 1035-1042.

- **Y. P. Zhang***, M. McDonnell, S. A. Calder and M. G. Tucker*. Mechanistic Insights into the Superexchange-Interaction-Driven Negative Thermal Expansion in CuO, *J. Am. Chem. Soc.*, 2019, **141**, 6310-6317.

- **Y. P. Zhang**, T. Scholz, R. Dronskowski*, M. McDonnell and M. G. Tucker*. Local magnetic cluster size identified by neutron total scattering in the site-diluted spin glass SnxFe4-xN (x=0.88). *Phys. Rev. B*, 2019, **100**, 014419.

- J. X. Hu*, T. H. Huang*, **Y. P. Zhang**, B. Hu, H. Q. Ye, B. J. Chen, H. P. Xia and C. Y. Ji. Enhanced deep-red emission from Mn4+/Mg2+ co-doped CaGdAlO4 phosphors for plant cultivation. *Dalton Trans.*, 2019, **48**, 2455-2466.

- J. X. Hu, **Y. P. Zhang**, H. P. Xia*, H. Q. Ye, B. J. Cheng and Y. S. Zhu. NIR Downconversion and Energy Transfer Mechanisms in Tb3+/Yb3+ Codoped Na5Lu9F32 Single Crystals. *Inorg. Chem.*, 2018, **57**, 7792-7796.

Professional Activities

Invited Talks:

- Y. P. Zhang, Probing local magnetic ordering with neutron total scattering. In: *MAGNA 2022*, Florida, US, May 1-4 , 2022.

- Y. P. Zhang, New development for neutron total scattering data reduction and analysis. In: *ACA Annual Meeting 2022*, Portland, US, Jul 29 - Aug 03 , 2022.

Community Support

- Our RMCProfile package for total scattering data modeling reached multiple milestones - 10, 000 downloads in total and 2, 000 downloads in one month for the first time.

- Peer reviewer for multiple journals including Physical Review Materials, Physica Status Solidi A, Ceramics International, etc.

Fundings

- Laboratory Directed Research & Development, Title: Automatic Structure Refinement Platform (ASRP) for neutron diffraction $217,000 10/7/2021, OAK RIDGE NATIONAL LABORATORY
- Laboratory Directed Research & Development, Title: Atomistic modeling and machine learning for neutrons $300,000 10/7/2021, OAK RIDGE NATIONAL LABORATORY

MENTORING

- Broud Michael, Title: Development of ADDIE web interface for neutron diffraction, Project: SULI 2023

- Paul Cuillier, Title: Probing the Origin of Fast Ionic Conduction in Li3YClxBr6-x Solid-State Electrolytes by Neutron Total Scattering and Hybrid Reverse Monte Carlo, Project: SCGSR 2022

- Jackson Wesley, Title: Post Processing Interface for ADDIE, Project: SULI 2022

- Caleb Chou, Title: Web Interface for Neutron Total Scattering Experiment Planning and Analysis, Project: SULI 2022

- Alexander D. Greenhalgh, Title: A New Data-Reduction Environment for Neutron Diffraction Data, Project: SULI 2021

AWARDS

- 2022 best paper 2022 of Neutron Scattering Division, Title: Hidden Local Symmetry Breaking in a Kagome-Lattice Magnetic Weyl Semimetal

SKILLS

Research:
- Total scattering (RMCProfile – *PR*, PDFgui – *PR*, Topas – *LP*) • Bragg refinement (GSAS – *PR*, Topas – *PR*) • EXAFS (Demeter – *PR*, FEFF – PR) • XANES (FEFF – *PR*, FDMNES – *PR*, FitIt – *PR*) • Molecular dynamics simulation (DL_POLY – *PR*, LAMMPS – *LP* , GULP – *BE*) • *ab initio* simulation (Quantum Espresso – *FA*, NWCHEM – *BE*).

Programming:
- Fortran (*PR*) • Python (script – *PR*, GUI development with wxpython – *PR*) • Bash script (*FA*) • LaTeX (*FA*) • Makefile (*FA*) • Mathematica (*FA*) • Matlab (including GUI dev, *LE*) • VisualBasic (*LE*) • C (*LE*) • C++ (*BE*) • Parallel programming with OpenMPI (in Fortran, *BE*) • GPU programming with CUDA (*BE*).

professional (*PR*) → *less professional* (*LP*) → *familiar* (*FA*) → *limited experience* (*LE*) → *beginner* (*BE*)

OTHER INTEREST/AMATEURS

- Developing little softwares/games. Here is a plane game that I developed using VB: Click Me!

- Diving into the ocean of open source softwares! Here is my desktop configured using the open source tool 'conky' under Ubuntu: Click Me! Here is an animation I produced with open source 3D modeling software Blender, demonstrating the Coriolis force: Click Me!