

Yuanpeng Zhang, PhD

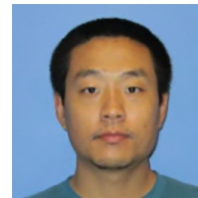
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SUMMARY

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

- Sichen Jiao, Yujian Sun, Dekai Shi, **Yuanpeng Zhang**, Xuelong Wang, Jue Liu*, Le Kang, Fangwei Wang, Xiqian Yu*, Hong Li*, Liquan Chen, Xuejie Huang*, *Energy Environ. Sci.* 2024, Advance Article.
- **Yuanpeng Zhang**, Zhiling Dun, Yunqi Cai, Chengkun Xing, Qi Cui, Naveen Kumar Chogondahalli Muniraju, Qiang Zhang, Yongqing Li, Jinguang Cheng*, and Haidong Zhou*, *Phys. Rev. B.* 2024, 109, 144407.
- Shumin Zhang, Feipeng Zhao, Lo-Yueh Chang, Yu-Chun Chuang, Zhen Zhang, Yuanmin Zhu, Xiaoge Hao, Jiamin Fu, Jiatang Chen, Jing Luo, Minsi Li, Yingjie Gao, Yining Huang, Tsun-Kong Sham, M. Danny Gu*, Yuanpeng Zhang*, Graham King*, and Xueliang Sun*, *J. Am. Chem. Soc.* 2024, 146, 5, 2977-2985.
- Hui Liu, Xiaoming Shi, Yonghao Yao, Huajie Luo, Qiang Li, Houbing Huang, He Qi, Yuanpeng Zhang, Yang Ren, Shelly D. Kelly, Krystian Roleder, Joerg C. Neufeind, Long-Qing Chen, Xianran Xing and Jun Chen. *Nat. Commun.*, 14, 1007 (2023).
- Zheng Sun, Ji Zhang, Huajie Luo, Yonghao Yao, Na Wang, Liang Chen, Tianyu Li, Changzheng Hu, He Qi, Shiqing Deng, Leighanne C. Gallington, **Yuanpeng Zhang**, Joerg C. Neufeind, Hui Liu*, and Jun Chen*. *J. Am. Chem. Soc.* 2023, 145, 11, 6194–6202.

- Yujian Sun, Sichen Jiao, Junyang Wang, Yuanpeng Zhang*, Jue Liu*, Xuelong Wang*, Le Kang, Xiqian Yu*, Hong Li, Liquan Chen, and Xuejie Huang. *J. Am. Chem. Soc.* 2023, 145, 21, 11717–11726.
- Deng Zhi, Chen Diacheng, Ou Mingyang, Zhang Yuanpeng, Xu Jia, Ni Dixing, Ji Zhaoran, Han Jiantao, Sun Yang, Li Shuai, Ouyang Chuying, Wang Zhaoxiang. *Adv. Energy Mater.*, 2023, 13, 2300695.
- Sichen Jiao, Yujian Sun, Junyang Wang, Dekai Shi, Yapei Li, Xiangkang Jiang, Fangwei Wang, Yuanpeng Zhang*, Jue Liu, Xuelong Wang, Xiqian Yu, Hong Li, Liquan Chen, Xuejie Huang, *Adv. Energy Mater.* 2023, 13, 2301636.
- **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. Neufeind, 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 Sr_xBa_{1-x}Nb₂O₆ (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 Sn_xFe_{4-x}N (x=0.88). *Phys. Rev. B*, 2019, **100**, 014419.

PROFESSIONAL ACTIVITIES

Invited Talks:

- Y. P. Zhang, RMCProfile: Big-box modelling of crystalline & amorphous materials, Budapest, Hungary, Sep 21, 2023.

- Y. P. Zhang, RMCProfile: Big-box modelling of crystalline & amorphous materials, Melbourne, Australia, Aug 21, 2023.
- 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

- Guest editor for *Materials* journal.
- Special issue editor for *Materials* journal.
- ICDD member of the Synchrotron & Neutron Scattering Methods Subcommittee.
- ICDD member of the Educational Subcommittee.
- 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: Software environment for Neutron Scattering Data Analysis, Interpretation and Automation \$422,000 10/7/2021, OAK RIDGE NATIONAL LABORATORY
- 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

- Dayton Kizzire, Title: Combination of exhaustive symmetry search and machine learning for phase transition studies. Project: NScD Postdoc Project.
- Pratanna Thamsorn, Title: Total scattering data denoising with autoencoder and convolutional neural network. Project: SULI 2024.
- Michael Broud, Title: Web interface for experimental planning at powder diffraction beamlines, Project: SULI 2023
- Paul Cuillier, Title: Probing the Origin of Fast Ionic Conduction in $\text{Li}_3\text{YCl}_x\text{Br}_{6-x}$ 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

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*, Web development with Flask – *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*) • Docker (*BE*) • Server DevOps (*BE*).

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

TRADEMARKS AND PATENTS

- ADvanced Diffraction Environment (ADDIE) in the cloud, addie.ornl.gov
- RMCProfile official website, rmcprofile.ornl.gov
- Powder diffraction documentation website, powder.ornl.gov
- Powder diffraction forum, powder.ornl.gov/forum
- Central Jupyter server for powder diffraction, powder.ornl.gov/hub

AWARDS

- 2022 NSD *Best Paper* Award.
- 2023 NSD *Doing it Better* Award.

OTHER INTEREST/AMATEURS

- Self hosting web services. Here is a dashboard that I created on my own cloud instance, <https://dh.iris-home.net/> which contains a full list of web services that I am hosting on my own VPS.
- 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!](#)