Curriculum Vitae

Xiaoping Wang, Ph.D.

Distinguished Scientist

Neutron Scattering Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6475, USA
Web: https://www.ornl.gov/staff-profile/xiaoping-wang

Email: wangx@ornl.gov
Office: 1(865)576-2148
Fax: 1(865)574-6080

ORCID: http://orcid.org/0000-0001-7143-8112

Scopus Author ID: 57202293130

Research Interests

Experimental and computational crystallography and structure-property relationships in materials through single crystal X-ray and neutron diffraction. Superspace approaches for modulated crystal data reduction and analysis. Instrumentation and software platforms at the ORNL Spallation Neutron Source leverage machine learning, artificial intelligence and high-performance computing to streamline data analysis across multidimensional diffraction and parameter spaces. Research focuses on structural and magnetic phase transitions, chemical and quantum crystallography, hydrogen-bonding networks in solids engineered for sustainable energy storage and carbon-capture applications.

Professional Experience

Lead Instrument Scientist - TOPAZ at the ORNL Spallation Neutron Source	2017 - present
Instrument Scientist - TOPAZ at the ORNL Spallation Neutron Source	2008 - 2017
Adjunct Professor, Department of Chemistry, University of North Texas	2007 - 2020
Director of X-ray Diffraction Laboratory, University of North Texas	2006 – 2008
Director of Crystallographic Computing, Laboratory for Molecular Structure and Bonding, Texas A&M University	2001 – 2006

Education/Training

Argonne National Laboratory	Neutron Diffraction	Postdoctoral	2000-2001
Texas A&M University	Inorganic Chemistry	Postdoctoral	1998-2000
Texas A&M University	Inorganic Chemistry	Ph.D.	1998
Nanjing University, China	Coordination Chemistry	M.S.	1990
Nanjing University, China	Chemistry	B.S.	1985

Honors and Awards

Fellow of the American Crystallographic Association – The Structure Science Society, 2019
ORNL's Top 10 Science Achievements at SNS and HFIR, 2023
ORNL's Top 10 Neutron Scattering Achievements, 2020
Supplemental Performance Awards, Oak Ridge National Laboratory, 2018
Significant Event Award, Oak Ridge National Laboratory, 2013
Supplemental Performance Awards, Oak Ridge National Laboratory, 2010
Outstanding Graduate Student, Texas A&M University, 1998
Welch Fellowship, Texas A&M University, 1996
Guanghua Scholarship, Nanjing University, 1990

Synergistic Activities

Co-Editor, IUCr Journal *Acta Crystallographica C, Structural Chemistry*, 2016 – present
Section Editor, *Crystals*, 2019 – present
Chair-Elect and Chair of the Small Molecule SIG, American Crystallographic Association, 2020, 2021

Professional Activities

Co-Organizer, MLXN 2025: Machine Learning for X-ray and Neutron Science, A Global 24-Hour Virtual Event, April 15, 2025
Organizer, Single Crystal Neutron Diffraction Data Reduction and Analysis, Oak Ridge National Laboratory, a satellite workshop at ACNS 2024, Knoxville, Tennessee, June 22, 2024
Organizer, Advanced Software Tools for Single Crystal Diffraction, A workshop at the American Crystallographic Association Annual Meeting, Portland, Oregon, July 29, 2022
Organizer, Advanced Software Tools for Single Crystal Data Analysis, an online workshop in the Joint Nanoscience and Neutron Scattering User Meeting, Oak Ridge, Tennessee, Aug. 2-3, 2021
Organizer, Workshop on Symmetry and Superspace Approach to Modulated Crystal Structures, Oak Ridge, Tennessee, Oct. 23-24, 2019
Member of the Program Committee for the 77 Pittsburg Diffraction Conference, and co-chaired the Small Molecule Crystallography Session, Oak Ridge, Tennessee, Oct. 24-26, 2019
Co-organizer TOPAZ Single Crystal Neutron Diffraction Workshop, Oak Ridge, TN, June 16-17, 2015
Scientific Session Organizer at various American Crystallographic Association Annual Meetings
Organizer and session chair, 'Public Domain Software', 2012 ACA Annual Meeting, Boston, MA, July 28 – August 1, 2012
Session Chair, 'Cool Structures', 2012 ACA Annual Meeting, Boston, MA, July 28 – August 1, 2012
Organizer and session chair, 'Materials for a Sustainable Future & Structure / Function of Metal-Organic Frameworks', 2013 ACA Annual Meeting, Honolulu, HI, Jul 20-24, 2013
Chair-Elect and Chair of the Small Molecule SIG, American Crystallographic Association, 2006,2007.
Panelist, NSF Science and Technology Center review committee, October 2012

Contribution to ORNL and Neutron Sciences

Developed a successful science program for single crystal neutron diffraction at TOPAZ
Established the workflow and user interface for single crystal neutron time-of-flight Laue data reduction.
Guided the development of software tools and user interface for single crystal experiment planning, data reduction and analysis
Provided guidance and performed McStas simulation for the successful commissioning and upgrade for TOPAZ
Provided recommendations to the post-audit committee as part of the NScD directorate-wide efforts for the improvement and growth of neutron facilities and the user program
Served on the Neutron Scattering Division Promotion Review Committee
Participated in Neutron Sciences Directorate committees on instrument post-audit, proposal reviews, and candidate interviews
Served on the ORNL LDRD SEED and science review committees
Mentoring graduate graduate students and postdocs at ORNL

Professional Affiliations

American Crystallographic Association – The Structural Science Society (Fellow 2019)
American Chemical Society
American Association for the Advancement of Science
Neutron Scattering Society of America

Selected Publications (from a list of 241 peer-reviewed journal articles, ***h***-index 50 on SciVal and 58 on Google Scholar. Full list of publications is available online at http://orcid.org/0000-0001-7143-8112)

Pawledzio S., Einkauf J., Custelcean R., Wang X.P., "Intermolecular Interactions in Direct Air Capture Materials: Insights from Charge Density Analysis", *Journal of the American Chemical Society,* (2025).

Xie Y., Koknat G., Weadock N.J., Wang X.P., Song R., Toney M.F., Blum V., Mitzi D.B., "Hydrogen Bonding Analysis of Structural Transition-Induced Symmetry Breaking and Spin Splitting in a Hybrid Perovskite Employing a Synergistic Diffraction-DFT Approach", *Journal of the American Chemical Society,* **146,** 22509–22521 (2024). DOE Highlight

Yin J., Reshniak V., Liu S., Zhang G., Wang X.P., Xiao Z., Morgan Z., Pawledzio S., Proffen T., Hoffmann C., Cao H.B., Chakoumakos B.C., Liu Y., "Integrated edge-to-exascale workflow for real-time steering in neutron scattering experiments", *Structural Dynamics,* **11,** 064303 (2024)

S.F. McWilliams, B.Q. Mercado, K.C. MacLeod, M.S. Fataftah, M. Tarrago, X.P. Wang, E. Bill, S. Ye, P.L. Holland, "Dynamic effects on ligand field from rapid hydride motion in an iron(ii) dimer with an S = 3 ground state", *Chemical Science,* **14,** 2303-2312 (2023). Highlighted by ORNL News, Featured in the *2023 Chemical Science HOT Article Collection* and *2023 ChemSci Pick of the Week Collection*

V. Elakkat, E. Tessema, C.-H. Lin, X. Wang, H.-C. Chang, Y.-N. Zheng, Y.-C. Huang, Gurumallappa, Z.-Y. Zhang, K. Long Chan, H. A. Rahayu, J. S. Francisco, and N. Lu, Unusual Changes of C−H Bond Lengths in Chiral Zinc Complexes Induced by Noncovalent Interactions, *Angewandte Chemie International Edition* **62**, e202215438 (2023). Selected for the 2023 NScD Top 10 Science Achievements

N. Lu, V. Elakkat, J. S. Thrasher, X. P. Wang, E. Tessema, K. L. Chan, R. J. Wei, T. Trabelsi, J. S. Francisco, Neutron Diffraction Study of Significant sp^3 and sp^2 C-H Bond Shortening in a Fluorinated Pyridinium Saccharinate. *Journal of the American Chemical Society* **143**, 5550-5557 (2021).

J. A. Smith, K. B. Wilson, R. E. Sonstrom, P. J. Kelleher, K. D. Welch, E. K. Pert, K. S. Westendorff, D. A. Dickie, X. Wang, B. H. Pate, W. D. Harman, Preparation of cyclohexene isotopologues and stereoisotopomers from benzene. *Nature* **581**, 288-293 (2020). ORNL News Neutrons – Deuterium shuffle | ORNL and selected for the ORNL's Top 10 Neutron Scattering Achievements of 2020 | Neutron Science at ORNL DOE Highlight

Custelcean, R.; Williams, N. J.; Wang, X. P.; Garrabrant, K. A.; Martin, H. J.; Kidder, M. K.; Ivanov, A. S.; Bryantsev, V. S., Dialing in Direct Air Capture of CO_2 by Crystal Engineering of Bisiminoguanidines. *Chemsuschem* **13** (23), 6381-6390 (2020). DOE Highlight

C. G. Gianopoulos, Z. Chua, V. V. Zhurov, C. A. Seipp, X. Wang, R. Custelcean, A. A. Pinkerton, Direct air capture of CO_2 - Topological analysis of the experimental electron density (QTAIM) of the highly insoluble carbonate salt of a 2,6-pyridine-bis(iminoguanidine), $(PyBIGH)_2(CO_3)(H_2O)_2$. *IUCrJ* **6**, 56-65 (2019). ORNL News Neutrons—Capturing carbon in mid-air | ORNL

B. Yang, W. Ming, M. H. Du, J. K. Keum, A. A. Puretzky, C. M. Rouleau, J. Huang, D. B. Geohegan, X. Wang, K. Xiao, Real-Time Observation of Order-Disorder Transformation of Organic Cations Induced Phase Transition and Anomalous Photoluminescence in Hybrid Perovskites. *Adv. Mater.* **30** (2018). Journal Cover, ORNL News Neutrons provide insights into increased performance for hybrid perovskite solar cells | ORNL and Neutron Science Highlight Neutrons Provide Insights into Increased Performance for Hybrid Perovskite Solar Cells | Neutron Science at ORNL DOE Highlight

Y. Ren, I. W. H. Oswald, X. Wang, G. T. McCandless, J. Y. Chan, Orientation of organic cations in hybrid inorganic-organic perovskite CH3NH3PbI3 from subatomic resolution single crystal neutron diffraction structural studies. *Cryst. Growth Des.* **16**, 2945-2951 (2016). Journal Cover. DOE Highlight

Invited Lectures

Recent Advances of Single Crystal Neutron Diffraction Data Reduction and Analysis at HFIR and SNS. Single Crystal Neutron Diffraction Data Reduction and Analysis Workshop, June 22, 2024, ACNS 2024.

Single Crystal Neutron Diffraction. UTK Physics Department, Knoxville, TN, February 28, 2023.

Software tools for neutron wavelength-resolved Laue diffraction in multidimensional diffraction and parameter spaces. American Crystallographic Association Annual Meeting, Portland, Oregon, August 1, 2022.

Recent Development in Single Crystal Neutron Diffraction. American Chemical Society 2022 Fall Meeting, Chicago, IL & Hybrid, August 23, 2022.

Crystal Engineering Turns on Direct Air Capture of CO_2. Emerging sample environment and neutron polarization needs for Chemistry, Geochemistry and Environmental Science Workshop. ORNL-NSD, May 11, 2022.

Direct Air Capture of CO_2. SMART FORUM and Crosscutting Initiative Meeting, ORNL-NSD, March 22, 2023.

Sample screening and alignment for single crystal neutron diffraction. Rigaku Single Crystal Online Users' Meeting, Woodland, TX, August 12, 2020.

Accurate hydrogen position from single crystal neutron diffraction. American Crystallographic Association 2019 Annual Meeting, Kentucky, July 20 -24, 2019.

Real time data collection in multidimensional diffraction and parameter spaces, American Crystallographic Association Annual Meeting, Toronto, Canada. July 20-24, 2018.

In Situ Single Crystal Neutron Diffraction Unveils the Link Between Hydrogen Bonding in an Organic-Inorganic Hybrid Perovskite and Its Anomalous Optoelectronic Property, MRS Spring Meeting, Phenix, AZ, April 5, 2018.

Transition path of organic cation induced anomalous photoluminescence in hybrid lead perovskites from real-time single crystal neutron diffraction, The 255th ACS National Meeting, New Orleans, LA, March 18-22, 2018.

Neutron Single Crystal Diffraction, Principle and Application in Chemistry and Materials Science. Open Guest Lecture, Department of Chemistry and Chemical Biology, Harvard University. April 6, 2017.

3D Single crystal diffraction at sub-atomic resolution: How this is done at the ORNL Spallation Neutron Source, American Crystallographic Association Annual Meeting, Denver CO. July 22-26, 2016.

Neutron single crystal diffraction study of hydrogen bonding in energy materials, Keynote speaker, The TWNSS Annual Meeting and Neutron Scattering Workshop, Huisun Forest of National Chung Hsing University, Taiwan, Oct. 21-23, 2016.

Octahedral tilting and cation ordering in topological insulators and hybrid photovoltaic materials revealed by single crystal neutron diffraction, Department of Physics, National Taiwan Normal University, Taipei, Taiwan, October 24, 2016.

Neutron single crystal diffraction study of hydrogen bonding in energy materials, Department of Chemistry, National Dong Hua University, Taiwan, October 26, 2016.

Single-crystal to Single-crystal Structural and Chemical Transformation of an Iron-based Molecular Electrocatalyst for Hydrogen Oxidation and Production. Philadelphia, PA, July 25-29, 2015.

Commissioning of the Neutron TOF Laue Single-Crystal Diffractometer TOPAZ at the Spallation Neutron Source, *The First Element - Transaction Symposium in memory of Bob Bau*, American Crystallographic Association Annual Meeting, Chicago, IL. July 24-29, 2010.

Selected Workshop Presentations & Lectures

Real-Time Mapping of Structural and Magnetic Phase Transitions with Neutron Wavelength-Resolved Laue Diffraction. American Physics Scociety March Meeting, Anaheim, California, March 18, 2025.

Integrated AI/ML and HPC Framework for Multidimensional Neutron Crystallography. American Crystallographic Association Annual Meeting, Denver, Colorado, July 11, 2024.

Processing of twinned and incommensurate data from neutron TOF Laue diffraction. Advanced Software Tools for Single Crystal Diffraction Workshop, American Crystallographic Association Annual Meeting, Portland Oregon, July 29, 2022.

Single-crystal diffraction beyond three dimensions: dynamic structural responses of hydrogen-bonded materials using time filtering of event-based neutron TOF Laue diffraction. American Crystallographic Association 2021 Annual Meeting Held Online, July 30 – August 5, 2021.

Cool structures from event-based single crystal neutron diffraction. American Crystallographic Association 2020 Annual Meeting Held Online, August 2-7, 2020.

Single crystal neutron diffraction beyond three dimensions. First Integrated Workshop on Neutron Diffuse Scattering from Single Crystals, June 6, Oak Ridge National Laboratory, Oak Ridge, TN, 2019.

Event based data collection for the TOPAZ beamline. WAND^2 Complementarity and Synergy Effects with JRR3 Instrument Suite Workshop, Knoxville, TN, July 14, 2019.

Single crystal neutron diffraction beyond three dimensions. Mantid Users Workshop, Grenoble, France, April 3–5, 2019.

Real time data collection in multidimensional diffraction and parameter spaces. American Crystallographic Association 2018 Annual Meeting, Toronto, Ont. Canada, July 20 – 24, 2018.

TOPAZ data reduction and analysis, Meeting of Experts for Single Crystal Diffraction Workshop, Data Management & Software Centre (DMSC) at European Spallation Source, Lund, Sweden, September 12, 2018.

Structure Analysis Using Neutron Data, A Mini-Workshop, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, April 7, 2017.

3D Single Crystal Diffraction at Sub-atomic Resolution: How This is Done at the ORNL Spallation Neutron Source. American Crystallographic Association 2016 Annual Meeting, Denver, CO, July 22 - 26, 2016.

Study of Hydrogen Bonding in Energy Materials Using Single Crystal Neutron Diffraction, ORNL/Georgia Tech Joint Workshop in Neutron Science and Scattering, Atlanta, GA, January 27, 2016.

Refinement of small molecules against neutron data, SHELX Workshop, Denver, CO, July 21, 2016.

Hydrogen in Materials -Structural study of an Fe-based electrocatalyst, Duke – ORNL Neutron Scattering Workshop, Duke University, Durham, NC, September 18, 2015.

Single-crystal to Single-crystal Structural and Chemical Transformation of an Iron-based Molecular Electrocatalyst for Hydrogen Oxidation and Production, American Crystallographic Association 2015 Annual Meeting, Philadelphia, PA, July 25 - 29, 2015.

Single crystal Neutron Diffraction, New York University Diffraction Workshop, New York, NY, Oct. 24-25, 2012.

Visualization of Guest-Host Interactions in Energy Storage Materials Using X-Ray and Neutron Diffraction Methods. American Crystallographic Association 2011 Annual Meeting, New Orleans, LA, May 28 - June 2, 2011.

Lecturer, National School on Neutron and X-ray Scattering, ORNL, 2008 – 2010.

Prepared experimental lectures and tutorial materials for ORNL Neutron School students and for training TOPAZ users, 2010 – present.