

# Curriculum Vitae

## Xiaoping Wang, Ph.D.

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### Neutron Scattering Division Oak Ridge National Laboratory

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### Current Position

Senior Neutron Scattering Scientist, SNS TOPAZ Point of Contact

### Education/Training

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

### Research and Professional Experience

- 2008 - present Instrument Scientist, SNS BL-12 TOPAZ at the Spallation Neutron Source  
TOPAZ Point of Contact since 2017, Senior Neutron Scattering Scientist since 2018.
- 2007 - 2020 Adjunct Professor, University of North Texas
- 2006 - 2008 Research Scientist, University of North Texas  
Director of the X-ray Diffraction Laboratory in the Department of Chemistry
- 2001 - 2006 Research Scientist, Texas A&M University  
Director of Crystallographic Computing in the Laboratory for Molecular Structure and Bonding at Texas A&M University

### Areas of Specialization

Single crystal neutron & X-ray diffraction, Inorganic chemistry, Energy materials, Instrumentation at large scale research facility.

## **Research Interests**

My primary research interest is applications of single crystal neutron and X-ray crystallography in chemistry and materials science. Research topics include hydrogen bonding in energy materials, metal hydride, guest-host interactions in metal-organic frameworks, magnetism, study structural phase transitions in multidimensional diffraction and parameter spaces.

## **Contribution to 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 for single crystal experiment planning, data reduction and analysis

Provided guidance and McStas simulation for the successful commissioning and upgrade for TOPAZ

Provided recommendations on the post-audit committee as part of the NScD directorate-wide efforts for the improvement and growth of the neutron facilities and user program.

Mentor, ORNL GO! Students

Participated in Neutron Sciences Directorate committees on instrument post-audit, proposal reviews, and candidate interviews.

## **Honors and Awards**

Fellow of the American Crystallographic Association, 2019

Outstanding Graduate Student, Texas A&M University, 1998

Welch Fellowship, Texas A&M University, 1996

Guanghua Scholarship, Nanjing University, 1990

## **Professional Activities**

Editorial Board Member, Crystals, 2019 – present.

Review Board Member, IUCr Journal Acta Crystallographica C, Structural Chemistry, 2016 – present

Chair-Elect and Chair of the Small Molecule SIG, American Crystallographic Association, 2020-2021.

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

Chair-Elect and Chair of the Small Molecule SIG, American Crystallographic Association, 2006-2007.

Panelist, NSF Science and Technology Center review committee, October 2012

Member of ORNL LDRD Seed Money Committee, May 2009 – May 2011

Member of TOPAZ Instrument Development Team 2003 - 2009

## Professional Affiliations

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

## Selected Publications (from a list of 195 peer reviewed journal articles, *h*-index 44)

1. N. Lu, V. Elakkat, J. S. Thrasher, X. Wang, E. Tessema, K. L. Chan, R. J. Wei, T. Trabelsi, J. S. Francisco, Neutron Diffraction Study of Significant sp<sup>3</sup> and sp<sup>2</sup> C-H Bond Shortening in a Fluorinated Pyridinium Saccharinate. *Journal of the American Chemical Society* **143**, 5550-5557 (2021).
2. 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**
3. C. G. Gianopoulos, Z. Chua, V. V. Zhurov, C. A. Seipp, X. Wang, R. Custelcean, A. A. Pinkerton, Direct air capture of CO<sub>2</sub> - Topological analysis of the experimental electron density (QTAIM) of the highly insoluble carbonate salt of a 2,6-pyridine-bis(iminoguanidine), (PyBIGH<sub>2</sub>)(CO<sub>3</sub>)(H<sub>2</sub>O)<sub>4</sub>. *IUCr* **6**, 56-65 (2019). ORNL News [Neutrons—Capturing carbon in mid-air | ORNL](#)
4. B. Yang, W. Ming, M. H. Du, J. K. Keum, A. A. Puzetky, 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**
5. Y. Ren, I. W. H. Oswald, X. Wang, G. T. McCandless, J. Y. Chan, Orientation of organic cations in hybrid inorganic-organic perovskite CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> from subatomic resolution single crystal neutron diffraction structural studies. *Cryst. Growth Des.* **16**, 2945-2951 (2016). Journal Cover, **DOE Highlight**

## Invited Lectures

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

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

*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, Apr. 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. Apr. 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, Oct. 24, 2016.

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

*Cool structures from event-based single crystal neutron diffraction*. The 70th American Crystallographic Association Annual (Virtual) Meeting, Aug. 2-7, 2020

*Event based data collection for the TOPAZ beamline. WAND<sup>2</sup> Complementarity and Synergy Effects with JRR3 Instrument Suite Workshop*, July 14, 2019, Knoxville, Tennessee.

*Single crystal neutron diffraction beyond three dimensions. First Integrated Workshop on Neutron Diffuse Scattering from Single Crystals*, June 6, 2019, ORNL.

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

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

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

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

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

Duke – ORNL Neutron Scattering Workshop, Duke University, Durham, NC, 2015.

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

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

Design instruction and tutorial materials for the Neutron School TOPAZ Experiments, 2014 – present.

**Graduate and Postdoctoral Advisor** F. Albert Cotton, Texas A&M University (Deceased)  
**Postdoctoral Advisors** F. Albert Cotton, Texas A&M University (Deceased)  
Arthur J. Schultz, Argonne National Laboratory