Curriculum Vitae

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Current Position

Senior Neutron Scattering Scientist

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

2017 – present Lead Instrument Scientist and Point of Contact, SNS BL-12 TOPAZ at the SNS
2008 - 2017 Instrument Scientist, SNS BL-12 TOPAZ at the SNS
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, Chemical crystallography, and 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, structural and magnetic phase transitions, hydrogen bonding interactions in functional materials for green energy and carbon capture applications.

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 for single crystal experiment planning, data reduction and analysis.

Provided guidance and 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.

Mentor of ORNL GO! students, postdocs.

Member of the Neutron Scattering Division Promotion Review Committee.

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

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

Professional Activities

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

Editorial Board Member, *Crystals*, 2019 – present.

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

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.

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 208 peer-reviewed journal articles, *h*-index 46. Full list of publications is available online at http://orcid.org/0000-0001-7143-8112)

1. 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).
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. 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

3. 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), (PyBIGH2)(CO3)(H2O)4. *IUCrJ* **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. 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

5. 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

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.

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.

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

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.

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