BRIAN H. TOBY

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RESEARCH INTERESTS

- Instrumentation and data analysis techniques for structural analysis from powder diffraction
- Crystallographic studies of functional metal oxides
- Non-periodic behavior (local distortions) in crystalline materials
- Informatics of powder diffraction and solid-state chemistry
- Molecular sieve structure-property relationships

EDUCATION

Ph.D., Physical Chemistry, California Institute of Technology, 1986
Thesis: Studies of Molecular Bonding, Interactions and Decomposition Reactions on the (001) Surface of Ruthenium, **Advisor:** W. Henry Weinberg

B.A., Chemistry, Rutgers College, 1980
Henry Rutgers Thesis: Studies in X-ray Crystallography, **Advisors:** Joseph A. Potenza and Harvey J. Schugar

PROFESSIONAL EXPERIENCE

Advanced Photon Source, Argonne National Laboratory, Physicist 2005-2008, Materials Characterization Group Leader 2006-2009, Senior Physicist 2008-, Section Head for Scientific Software, 2009-2015, Computational X-ray Science Group Leader and APS Chief Computational Scientist 2015-.

NIST Center for Neutron Research, Research Chemist 1995-2005, Crystallography Team Leader 1998-2005.

Air Products and Chemicals, Inc., Central Research Services Dept., Principal Research Chemist, 1991-1993, Senior Principal Research Chemist 1993-1995.

University of Pennsylvania, Department of Materials Science and the Laboratory for Research on the Structure of Matter, Research Associate, 1988-1990, Lecturer 1990-1991. **Supervisor:** Takeshi Egami

Union Carbide, Corp., Central Scientific Lab., Senior Chemist, 1985-1988.

HONORS

Co-recipient (with Robert Von Dreele) of the 6th American Crystallographic Association Ken Trueblood Award for "exceptional achievement in computational or chemical crystallography." (2019)

Fellow, American Crystallographic Association (2017)

16th recipient of the Charles S. Barrett Award from the Denver X-ray Conference for outstanding contributions to the field of powder diffraction (2015)

Elected as chair to U.S. National Committee for Crystallography, National Academy of Science (2012-2014)

Bronze Medal from U.S. Department of Commerce for "Contributions to Powder Diffraction Software" (2005)

Fellow, International Centre for Diffraction Data (2004)

Phi Beta Kappa (1980)

American Institute of Chemists Undergraduate Award (1980)

B.A. awarded with Highest Distinction in Chemistry and with Honors (1980)

PROFESSIONAL SERVICE

American Crystallographic Association:

Vice-President (2019), President (2020), Past-President (2020). Served as chair of the Nominations Committee and multiple Scientific Interest Groups. Member since 1989.

U.S. National Committee on Crystallography:

Member (2004-2006, 2007-2009), Vice Chair (2009-2011), Chair (2012-2014).

US Delegation Leader to the 23rd Congress of the International Union of Crystallography, 2014 (Montreal, Canada).

Elected as US Delegate to the 22nd Congress of the International Union of Crystallography, 2011 (Madrid, Spain).

Elected as US Delegate to the 21th Congress of the International Union of Crystallography, 2008 (Osaka, Japan).

Elected as US Delegate to the 20th Congress of the International Union of Crystallography, 2005 (Florence, Italy).

International Union of Crystallography memberships:

Committee on the Crystallographic Information File, 2000-2002; Commission on Neutron Scattering, 2008-2011; Commission on Powder Diffraction, 2010-2018.

Denver X-ray Conference:

Organizing committee member, 2008-.

Argonne-Oak Ridge Neutron/X-ray Summer School, Co-Director 2015-2020.

EDITORIAL ACTIVITIES

Editor for Crystallographic Education, *Powder Diffraction* journal (International Centre for Diffraction Data), 2006-. Editor of special issues for December 2011 and December 2014 on powder diffraction software.

Editorial Board, *The Journal of Physical and Chemical Reference Data*, 2007- (AIP/NIST)

Member, Publications Committee, American Institute of Physics, 2009-2012

Associate Editor, International Tables for Crystallography, Volume G (2005)

Editor, "Accuracy in Powder Diffraction III – Part 1", *J. Res. Natl. Inst. Stand.*, **109**(1)**,** (2004)

SIGNIFICANT TECHNICAL ACCOMPLISHMENTS

Software for analysis of Powder Diffraction: Co-author of the GSAS-II comprehensive crystallographic analysis package. Solo author of EXPGUI, a user-friendly interface to the General Structure Analysis System (GSAS) software package (cited ~5000 times.) Author of numerous crystallographic utility programs including CMPR, pdCIFplot and Powder Suite.

Construction and commissioning of the 11-BM high-resolution and high-throughput powder diffractometer: Scientific lead for the construction and commissioning for the first robotically-controlled high-resolution ($\Delta Q/Q < 2\times10^{-4}$) powder diffractometer in the US. Designed and implemented mail-in sample management and instrument control systems that redefine the state of the art to reduce staffing requirements, and provide for productivity tracking and sample disposal. Result: 11-BM has become the highest-publishing beamline in the APS, despite having only minimal staffing and only a bending magnet source.

Development of user program for the BT-1 neutron powder diffractometer: Pioneered use of Web for proposal submission, user outreach and data monitoring; established rapid review/scheduling cycle; expanded operation range of instrument to include more rapid data collection and high-Q operation. Result: BT-1 has the highest publication record of any thermal neutron instrument at NIST.

Informatics for powder diffraction: Extended the IUCr's Crystallographic Information File (CIF) electronic standard for exchange of crystallographic results to powder diffraction data.

Accomplishments: defined powder diffraction data dictionary; implemented software for archival of Rietveld refinement data and results within GSAS; created tool for editorial/referee review of Rietveld results; assisted editorial office with policy development for publication of powder diffraction results in the *Acta Crystallographia/Journal of Applied Crystallography*.

Derivation of error analysis for the pair distribution function: The pair distribution function (PDF) is used for analysis of local structure in nominally crystalline materials ("total scattering"). Error analysis was developed so that statistical error estimates of parameters from models fit to a PDF can be derived in a manner equivalent to that for conventional crystallographic results.

First Development of PDF Fitting for Crystalline Materials: To find local distortions in high-T_c superconductors, the first compact atomistic model fitting was performed to explain differences between the observed PDF and that which was predicted from the long-range crystal structure.

PUBLICATIONS

>140 refereed publications with >11,000 citations (h-index 40).
See http://www.researcherid.com/rid/F-3176-2013 or http://orcid.org/0000-0001-8793-8285

Postdoctoral scientists supervised, with most recent known position

Sytle Antao (Assistant professor, University of Calgary)
Camille Y. Jones (Assistant professor, Hamilton College)
Tammy Amos (Central Research, DuPont)
So-Hyun Park (completed Habilitation, Max Plank Institute)
Barbara A. Reisner (Full professor, James Madison University)
Roberto Senesi (Research staff, Instituto Nazionale di Fisica Nucleare)
Nazy Khosrovani (Accerlys, Inc.)

Undergraduate students supervised, with most recent known degree

Todd Zeitler (Ph.D. in Ceramics, Alfred University, 2006)
Michael Yurievich Polyakov (M.S. in Computer Science, Harvard University, 2006)
Caitlin Horn (B.A. expected 2021, Washington University of St. Louis)
Keara Ginell (B.A. expected 2022, Vassar College)