Bruce Ravel

Employment History

2008–present **Physicist**, *National Institute of Standards and Technology*, Gaithersburg MD, USA.
Synchrotron Methods Group at the National Synchrotron Light Source
Materials Measurement Science Division, Material Measurement Laboratory

2005–2008 **Assistant Physicist**, *Argonne National Laboratory*, Argonne IL, USA.
Molecular Environmental Science Group, Biosciences Division
Staff Scientist at The Materials Research Collaborative Access Team at the Advanced Photon Source

2001–2005 **Assistant Physicist**, *Naval Research Laboratory*, Washington, DC, USA.
Chemistry Division
Spokesperson for NSLS Beamlines X11A, X11B, X23B

2000–2001 **Postdoctoral Fellow**, *Naval Research Laboratory*, Washington, DC, USA.
Fellowship sponsored by The American Society of Electrical Engineers
Research Project: XAFS Studies of Half-Metallic Heusler Alloys

1999–2000 **Visiting scientist**, *Centre National de la Recherche Scientifique*, Grenoble, France.
Research Project: Diffraction Anomalous Fine Structure Investigation of Superlattice Reflections in $La_{1/3}Ca_{2/3}MnO_3$
Staff member at European Synchrotron Radiation Source beamline BM02

1997–1999 **Postdoctoral Fellow**, *National Institute of Standards and Technology*, Gaithersburg, MD, USA.
Fellowship sponsored by the National Research Council
Research Project: Diffraction Anomalous Fine Structure Investigation of the Ferroelectric Phase Transitions of $BaTiO_3$

Education

1991–1997 **PhD, Physics**, *University of Washington*, Seattle, WA.
Thesis title: Ferroelectric Phase Transitions in Oxide Perovskites Studied by XAFS
Advisers: Dr. Edward A. Stern and Dr. John J. Rehr

1989–1991 **MS, Physics**, *University of Washington*, Seattle, WA.

1985–1989 **BA, Physics**, *Wesleyan University*, Middletown, CT.

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Research Interests

XAS Method Development

XAS Data Analysis Software

I am a co-author of the widely used IFEFFIT analysis package. My contributions include the graphical user interfaces ATHENA (XAS Data Processing), ARTEMIS (EXAFS Data Analysis), and HEPHAESTUS (a periodic table for the X-ray absorption spectroscopist) as well as extensive documentation and training materials. Several times each year, I teach XAS training courses at synchrotrons and other institutions around the world.

The publication introducing ATHENA, ARTEMIS, and HEPHAESTUS has over 1800 citations as of May, 2013, making it the highest cited article in the Journal of Synchrotron Radiation.

Inform XAS analysis using local structure theory

Local structural theories – such as molecular dynamics, Monte Carlo, and others – show that common materials exhibit substantial local disorder that, in many cases, is poorly approximated by a simple cumulant expansion. I have ongoing projects involving metallic nanoparticles and other highly disordered materials to explore how careful consideration of non-cumulant local disorder can be modeled in EXAFS analysis, including contributions of disorder to multiple scattering paths.

Integrative beamline technologies

The advent of NSLS-II offers a rare opportunity to reconsider every aspect of beamline design and operation. I am interested in finding common frameworks for handling all aspects of an XAS beamline, including controls, diagnostics, data acquisition, data processing, and data archiving. The state of a beamline – that is, the state of all controls, diagnostics, and acquisition instrumentation – can be recorded continuously using scalable database technologies. This complete record of state can be integrated into a data archiving strategy and inform automated or other sophisticated data processing strategies.

Beamline Development

NSLS X23A2

I am the local contact at NIST's hard X-ray spectroscopy beamline with responsibilities that include user support, beamline maintenance, and scientific collaboration with beamline users. My recent instrumentation developments include development of accurate dead-time correction for silicon drift detectors and its integration into ATHENA, the development of a novel four-channel ionization chamber for parallel measurement of four XAS spectra, and the development of polycapillary lenses for X-ray spectroscopy applications.

NSLS-II BMM

With Joe Woicik, I am leading development of NIST's XAS and XRD beamline at NSLS-II. The *Beamline for Materials Measurement* will be on a 3-pole wiggler source. With new optics, the performance of this new beamline will vastly exceed that of X23A2. I am involved in all aspects of design and development and am interested in the development of novel control and data acquisition systems.

NSLS-II ISS

I was the spokesperson for the *Inner Shell Spectroscopy* beamline development proposal for NSLS-II. ISS was selected as one of the 6 NEXT beamlines currently and is currently approaching the final design phase. I am the chair of the Beamline Advisory Team (BAT), an international group of spectroscopy experts advising the ISS development team on all aspects of the technical plan and the scientific program. I am working with the ISS team to develop a prototype of the novel X-ray spectrometer planned for the beamline which will deliver XAS on low concentration or low volume samples, high resolution fluorescence detection, core and valence band X-ray emission spectroscopy, and X-ray energy loss spectroscopy.

XAS Training Courses (37)

- National Synchrotron Light Source, Nov. 8-10, 2012
- State University of New York at Binghamton, Oct. 25-26, 2012
- Karlsruhe Institute of Technology, Germany, Sep. 13-14, 2012
- Synchrotron Light Research Institute, Khorat, Thailand, Aug. 13-15, 2012
- Diamond Light Source, Nov. 14-16, 2011
- National Synchrotron Light Source, Nov. 3-5, 2011
- University of Ghent, Ghent Belgium, Jan. 12-14, 2011
- National Synchrotron Light Source, Nov. 4-6, 2010
- Johnson-Matthey Research Centre, Reading, England, Oct. 11-13, 2010
- Synchrotron Light Research Institute, Khorat, Thailand, Aug. 4-6, 2010
- University of Ghent, Ghent Belgium, Jan. 13-15, 2010
- National Synchrotron Light Source, Oct. 22-24, 2009
- Advanced Photon Source, July 6-10, 2009
- Synchrotron Light Research Institute, Khorat, Thailand, May 27-29, 2009
- National Synchrotron Light Source, Oct. 30 - Nov. 1, 2008
- Swiss Light Source, Paul Scherrer Institute, Switzerland, Oct. 8-10, 2008
- Canadian Light Source, Saskatoon, Saskatchewan, Canada, Aug. 20, 2008
- Advanced Photon Source, Aug. 4-8, 2008
- Advanced Photon Source, July 23-27, 2007
- Physics Institute of the Polish Academy of Science, Warsaw, Nov. 13-15, 2006
- Advanced Photon Source, July 26-28, 2006
- Swiss Light Source, Paul Scherrer Institute, Switzerland, Feb. 20-21, 2006
- Advanced Photon Source, July 26-29, 2005
- Michigan State University, Jan. 20-21 , 2005
- Canadian Light Source, Nov. 16-17, 2004
- National Synchrotron Light Source, June 22-25, 2004
- National Synchrotron Light Source, July 14-17, 2003
- Alberta Synchrotron Institute, Nov. 12-14, 2002
- National Synchrotron Light Source, Sep. 23-25, 2002
- National Synchrotron Light Source, June 27-29, 2001
- LNLS, Campinas, Brazil, May 7-9, 2001
- University of Seville, Spain, May 24-26, 2000
- CNRS, Grenoble France, May 17-19, 2000
- University of Wuppertal, Germany, June 13-15, 2000
- University of Leuven, Belgium, May 2-4, 2000
- ESRF, Grenoble France, March 15-17, 2000
- The Dow Chemical Company, Sep. 16-17, 1996

Online XAS training materials

Presentations viewable at https://speakerdeck.com/bruceravel
Training materials website at http://bruceravel.github.com/XAS-Education/

Language Skills

Spanish **Proficient** *I first learned Spanish as a child living in Costa Rica and have maintained proficiency as an adult.*

French **Conversational** *My French vocabulary is focused on a professional context due to my year working in Grenoble.*

References

Supervisor

Daniel Fischer
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Professional References

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John J. Rehr
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University of Washington, Seattle, WA 98195-1560, USA
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Significant Publications

ATHENA and ARTEMIS — Ravel, B. & Newville, M. ATHENA and ARTEMIS: data analysis for X-ray absorption spectroscopy using IFEFFIT, *Journal of Synchrotron Radiation* **12**, 537–541 (2005) doi:10.1107/S0909049505012719

FEFF8 — Ankudinov, A. L., Ravel, B., Rehr, J. J., Conradson, S. D., Real-space multiple-scattering calculation and interpretation of x-ray-absorption near-edge structure, *Physical Review B* **58**, 7565–7576 (1998). doi:10.1103/PhysRevB.58.7565

XAS Review — Kelly, S., Hesterberg, D. & Ravel, B., Analysis of soils and minerals using x-ray absorption spectroscopy, In Drees, L. & Ulery, A. (eds.) *Methods of Soil Analysis - Part 5: Mineralogical Methods*, chap. 14, American Society of Agronomy (2008) Science Societies bookstore

Publications

[1] Bruce Ravel. Path aggregation techniques for exafs visualization and analysis. *Journal of Physics: Conference Series*, 430(1):012006, 2013.

[2] Stephen W T Price, Nicholas Zonias, Chris-Kriton Skylaris, Andrea E Russell, and Bruce Ravel. The application of molecular dynamics to fitting exafs data. *Journal of Physics: Conference Series*, 430(1):012009, 2013.

[3] Daniel M. Pajerowski, Brian M. Zakrzewski, and Bruce Ravel. X-ray structural studies of prussian blue analog heterostructures on poly(ethylene terephthalate) supports. *Thin Solid Films*, 526(0):34 – 40, 2012.

[4] B. Ravel, J. R. Hester, V. A. Solé, and M. Newville. Towards data format

standardization for X-ray absorption spectroscopy. *Journal of Synchrotron Radiation*, 19(6):869–874, Nov 2012.

[5] Andrew S. Madden, Andrew L. Swindle, Melanie J. Beazley, Ji-Won Moon, Bruce Ravel, and Tommy J. Phelps. Long-term solid-phase fate of co-precipitated U(VI)-Fe(III) following biological iron reduction by Thermoanaerobacter. *American Mineralogist*, 97(10):1641–1652, October 2012.

[6] Stephen W. T. Price, Nicholas Zonias, Chris-Kriton Skylaris, Timothy I. Hyde, Bruce Ravel, and Andrea E. Russell. Fitting EXAFS data using molecular dynamics outputs and a histogram approach. *Phys. Rev. B*, 85:075439, Feb 2012.

[7] Christopher J. Patridge, Cherno Jaye, Tesfaye A. Abtew, Bruce Ravel, Daniel A. Fischer, Amy C. Marschilok, Peihong Zhang, Kenneth J. Takeuchi, Esther S. Takeuchi, and Sarbajit Banerjee. An X-ray Absorption Spectroscopy Study of the Cathodic Discharge of $Ag_2VO_2PO_4$: Geometric and Electronic Structure Characterization of Intermediate phases and Mechanistic Insights. *J. Phys. Chem. C*, 115(29):14437 – 14447, 2011.

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[11] Christopher J. Patridge, Tai-Lung Wu, Cherno Jaye, Bruce Ravel, Esther S. Takeuchi, Daniel A. Fischer, G. Sambandamurthy, and Sarbajit Banerjee. Synthesis, spectroscopic characterization, and observation of massive metal-insulator transitions in nanowires of a nonstoichiometric vanadium oxide bronze. *Nano Letters*, 10(7):2448 – 2453, 2010.

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spectra from around the world. *Journal of Physics: Conference Series*, page 012032 (4 pp.), 2009.

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