**DANIEL OLDS**

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## RESEARCH INTERESTS

My research focus lies in combining diffraction techniques with *in situ* studies of complex materials to discover the underlying atomic origins of the relevant material properties, such as reaction pathways, decomposition mechanisms, phase-transitions, and material passivation/poisoning. I approach these challenging scientific problems with expertise in three areas: detail-oriented design of advanced sample environments optimized for neutron diffraction, experience with a wide variety of conventional analysis tools, and the ability to develop custom data reduction and analysis methods to meet specific needs found through 'at the beamline' experiences.

## CAREER

Oak Ridge National Laboratory **2015-Present**
**Postdoctoral Researcher in Neutron Diffraction and PDF**
Postdoc Mentor: Katharine Page

Los Alamos National Laboratory
**Postdoctoral Researcher and Instrument Assistant on Low-Q Diffractometer** **2013-2015**
Postdoc Mentor: Rex Hjelm

## EDUCATION

Michigan State University
**Ph.D. in Physics** **2008-2013**
Thesis Topic : "Refinement of simulated polymer-fullerene photovoltaic devices through small angle scattering and dynamic Monte Carlo"
Thesis Advisor : Philip Duxbury

Michigan State University **2005-2008**
**M.S. in Physics**

Michigan State University **2001-2005**
**B.S. in Physics**

## PUBLICATIONS

Daniel Olds, Marshall McDonnell, Katharine Page, Peter F. Peterson – *"Unified conversions between total scattering data formalisms"*, Acta Crystallographica A, **In Prep** **2018**

Tedi-Marie Usher, Daniel Olds, Jue Liu, and Katharine Page - *"A numerical method for deriving shape function of nanoparticles for pair distribution function refinements",* Acta Crystallographica A, **In Review** **2018**

Arne Peys, Claire White, Daniel Olds, Huber Rahier, Bart Blanpain, and Yiannis Pontikes -*"Molecular structure of CaO-$FeO_x$-$SiO_2$ glassy slags and resultant inorganic polymer binders",* Journal of Physical Chemistry C, **In Review** **2018**

Daniel Olds, Claire N. Saunders, Megan Peters, Thomas Proffen, Joerg Neuefeind, and Katharine Page - *"Precise implications on real-space PDF modeling from effects intrinsic to modern time of flight neutron diffractometers",* Acta Crystallographica Section A, **Accepted as Feature Article** **2018**

Daniel Olds, Keith V. Lawler, Arnold A. Paecklar, Jue Lue, Katharine Page, Peter F. Peterson, Paul M. Forster, and James R. Neilson - *"Capturing the details of N2 adsorption in zeolite X using stroboscopic isotope contrasted Neutron total scattering",* Chemistry of Materials, **30(1)**, 296-302 **2018**

Zhenduo Wu, Si Lan, Xiaoya Wei, Katharine Page, Daniel Olds, Baolong Shen, and Xun-Li Wang - *"Heterogeneous nucleation in Zr-Cu-Al-Ag metallic glasses triggered by quenched-in metastable crystals - a time-resolved neutron diffraction study",* Physica Scripta B, **92(11),** 114002 **2017**

Daniel Olds, Peter F. Peterson, Michael Crawford, James R. Neilson, Hsiu-Wen Wang, Pamela S. Whitfield, and Katharine Page - *"Combinatorial appraisal of transition states for in situ pair distribution function analysis"* Journal of the Applied Crystallography, **50(6)** **2017**

Douglas H. Fabini, Ting Ann Siaw, Constantinos C. Stoumpos, Geneva Laurita, Daniel Olds, Katharine Page, Jerry G. Hu, Merouri G. Kanatzidis, Songi Han, and Ram Seshadri – *"Universal Dynamics of Molecular Reorientation in Hybrid Lead Iodide Perovskites"* Journal of American Chemical Society, **139 (46)**, 16875–16884, **Journal Cover** **2017**

Heinz Nakotte, Corinne Silkwood, Katharine Page, Hsiu-Wen Wang, Daniel Olds, Boris Kiefer, Sohini Manna, Dmitry Karpov, Edwin Fohtung, and Eric E. Fullerton - *"Pair distribution function analysis applied to decahedral gold nanoparticles",* Physica Scripta, **82**, 11 **2017**

Jue Liu, Daniel Olds, Rui Peng, Lei Yu, Guo Shiou Foo, Shuo Qian, Jong Keum, Beth S. Guiton, Zili Wu, and Katharine Page - *"Quantitative analysis of the morphology of 101 and 001 faceted anatase TiO2 nanocrystals and its implications on photocatalytic activity",* Chemistry of Materials, **29**, 5591-5604 **2017**

Daniel Olds, Katharine Page, Arnold Paecklar, Peter F. Peterson, Jue Liu, Gerald Rucker, Mariano Ruiz-Rodriguez, Michael Olsen, Michelle Pawel, Steven H. Overbury, and James R. Neilson - *"A high precision gas flow cell for performing in situ neutron studies of local atomic structure in catalytic materials",* Review of Scientific Instruments, **88**, 034101 **2017**

Claire E. White, Daniel Olds, Monika Hartl, Rex P. Hjelm, and Katharine Page - *"Evolution of the pore structure during the early stages of the alkali-activation reaction: an in situ small-angle neutron scattering investigation",* Journal of Applied Crystallography, **50**, 61-75 **2017**

Hsiu-Wen Wang, Luke L. Daemen, Michael C. Cheshire, Michelle K. Kidder, Andrew G. Stack, Lawrence F. Allard, Jorg Neuefeind, Daniel Olds, Jue Liu, and Katharine Page - *"Synthesis and structure of synthetically pure and deuterated amorphous (basic) calcium carbonates",* Chemical Communications, **53**, 2942-2945 **2017**

Monika Hartl, Robert Chad Gillis, Luke Daemen, Daniel Olds, Katharine Page, Stefan Carlson, Yongqiang Cheng, Thomas Huegle, Erik B. Iverson, A. J. Ramirez-Cuesta, Yongjoong Lee, and Gunter Muhrer - *"Hydrogen adsorption on two catalysts for the ortho- to parahydrogen conversion: Cr-doped silica and ferric oxide gel",* Physical Chemistry Chemical Physics, **18**, 17281 **2016**

Daniel Olds, Hsiu-Wen Wang, and Katharine Page - *"DShaper: an approach for handling missing low-Q data in pair distribution function analysis of nanostructured systems",* Journal of Applied Crystallography, **48**, 1651-1659 **2015**

Sarah Barnhill, Nia Bell, Joseph Patterson, Daniel Olds, and Nathan Gianneschi - *"Phase diagrams of polynorbornene amphiphilic block copolymers in solution*", Macromolecules, **48**, 48(4), 1152-1161 **2015**

Daniel Olds, Philip Duxbury - *"Efficient algorithms for calculating small angle scattering from large model structures",* Journal of Applied Crystallography, **47**, 1077 **2014**

Daniel Olds - *"Refinement of simulated polymer-fullerene photovoltaic devices through small Angle scattering and dynamic Monte Carlo",Doctoral dissertation, Michigan State University* **2013**

Daniel Olds, Jon Kiel, Michael Mackay, Philip Duxbury - *"Percolating bulk-heterostructures from neutron reflectometry and small angle scattering data",* Physical Review E, **86**, 061803 **2012**

## PRESENTATIONS

*"Correlating the chronology and local structure of energy materials"* **2017**
24th Congress and General Assembly of the International Union of Crystallography – Hyderabad, India

*"Improving the accuracy of time of flight neutron total scattering data analysis"* **2017**
American Crystallographic Association – New Orleans (LA)

*"An In Situ Gas Flow Cell for Stroboscopic Studies of Local Atomic Structure in Catalytic Materials",* American Conference on Neutron Scattering – Long Beach (CA) **2016**

*"Bridging the lengthscales : From before the Bragg Peaks to Beyond"* **2015**
American Crystallographic Association – Philadelphia (PA)

*"Porosity of ceramic UO2 in nuclear fuel rods under extreme conditions"* ***2014***
NuMat : The Nuclear Materials Conference - Clearwater (FL)

*"MaxEnt : A length scale bridge for multiscale nanomaterials"* ***2014***
American Conference on Neutron Scattering - Knoxville (TN)

*"Stroboscopic probes of transient response to time dependent stresses in soft condensed matter"* ***2014***
American Crystallography Association Meeting - Albuquerque (NM)

*"Percolating bulk-heterostructures from neutron reflectometry and small angle scattering data"* ***2013***
American Physical Society March Meeting - Baltimore (MD)

*"The effect of morphology on charge transport in OPV Devices"* ***2011***
Complex Materials for Energy Applications Seminar – East Lansing (MI)

*"Continuum and KMC simulations of realistic bulk heterostructure solar cell photovoltaic devices"*
American Physical Society March Meeting - Portland (OR) **2010**

## AWARDS AND HONORS

Recipient of 2017 Etter Student Award from Neutron Scientific Interest Group at the 2017 American Crystallographic Association Meeting for *"Improving the accuracy of time of flight neutron total scattering data analysis"* – New Orleans (LA) **2017**

Poster Prize Awarded at RMCProfile School for "*DShaper - A program to efficiently handle the effects of missing low-Q data in pair distribution function analysis of nanostructured systems*" – Oak Ridge (TN) **2016**

## SKILLS AND PROGRAMS

**Experimental Skills**

Expertise in many different scattering techniques, including Bragg diffraction, Pair-distribution Function (PDF) methods, small angle scattering, and reflectometry.

Significant experience on many different beamlines, both with neutrons (SNS: NOMAD, POWGEN; HFIR: BIO-SANS; and Lujan Center: NPDF, LQD, SPEAR) and synchrotron X-ray (APS: 11-IDB, 5-ID)

Experience with Residual gas analysis (RGA) via Altamira AMI-300 Reactor, Stanford Research Systems UGA-200, and home-built high precision gas flow cell (see associated publication).

Experience with general chemistry lab work (basic synthesis, sample prep, glovebox work, XRD, ect.)

**Programming Skills**
Proficient in Python, Fortran, C++, MATLAB, MATHEMATICA, IGOR Pro, and IDL.

Demonstrated success in delivering user-focused GUI-driven software and prototypes.

Experience with a wide variety of analysis software for scattering data, such as TOPAS, GSAS, PDFgui, Discus, Motofit, Irena, NCNR Macros, PDF-4, and SASView.

Have developed tools which can be incorporated into modeling efforts of Discus and TOPAS, available online at www.github.com/DanOlds/

Maintain a detailed library of 'peak-shape' simulation effects, as they relate between real and reciprocal space representations of data. Expert on details of Fourier transform, and associated analysis methods (filtering, aberration mitigation, hierarchical analysis).

Developed a series of simple tutorials to teach users about total scattering data reduction, towards an optimized PDF.

**Software Projects**
*RosettaPDF* – Neural network trained to recognize, and convert between, the different forms of total scattering data employed by the worldwide community.

*ADDIE* – The advanced diffraction data reduction environment, currently deployed on NOMAD as primary data reduction framework.

*CATS* – Software/GUI to perform model free analysis using a new machine learning algorithm I developed (Combinatorial Appraisal of Transition States) to study systems undergoing phase-changes or feature tracking, when end-states are known *a priori*.

*FastGR* – An extreamly user friendly program to aid with optimization of PDF data, which was the precursor to and has since spun up into the fully supported ADDIE total scattering data reduction environment.

*Driver* - Easy-to-use rapid scripting of more complex total scattering and diffraction analysis programs (i.e. Topas, Discus) via a simple Jupyter notebook framework.

*DShaper* – A method and program to approximate characteristic shape functions from atomistic models, useful in PDF studies of materials with nanoscale structure.

*MaxEnt* – A method to simultaneously and coherently reduce data from small angle scattering and powder-diffraction based PDF into a single dataset through Bayesian methods.

*Strobosim* – A code which examines the effect of choppers on the pulse structure, in time and energy, of a neutron pulse at a spallation source flightpath. This code, used in conjunction with the neutron instrument simulation package (NISP, McSTAS), explores the feasibility of stroboscopic techniques at a flightpath.

*Slimscatter* – A highly optimized code to efficiently simulate SAS data from a large box atomistic model using Monte Carlo sampling of the Debye approach.

*MakeIsing* – A verbose and user friendly code to generate 3D two-phase morphologies which are then annealed via a modified form of the Ising model. The input which drives the ultimate structure incorporate SAS and reflectometry data.

*Helios* – A morphology driven device simulator for organic photovoltaic devices. This code simulates a wide variety of behaviors in OPV systems on models provided by the user, which allows for examination of the effect nanoscale morphology plays on overall device performance.

**Other Expertise and Skills**

Experience with the design and operation of a diverse set of sample environments for use in small angle, diffraction, and total scattering measurements including a high pressure cell, gas flow cell, tensile load frame, polymer shear cell, vacuum furnace, electrochemical cell, photovoltaic rig, reactor cell, RF furnace, and high-throughput sample changer.

Strong collaborative skills which have led to the development of research independent of my advisor and mentor directed projects.

Experience as an instrument assistant on a user program beamline with responsibilities including maintenance and operation of software and hardware, sample synthesis and preparation, user instruction in data collection and analysis, data reduction, and regular periods of 24 hour on call support.

Demonstrated ability to bootstrap a project from the initial stages of development to successful publication.

Held a DOE Q-clearance for work at Los Alamos National Laboratory from 2014 – 2015.

## TEACHING EXPERIENCE

Oak Ridge National Laboratory

**Beamline User Training and Assistance** **2016-2018**

Act as local contact for selected external beamline users. Assisted in proposal inception and writing, at-the-beamline training, general technique education, and materials specific analysis instruction.

**Summer School Instructor** **2016-2017**

Presented lectures and provided assistance during hands-on tutorials for a series of summer schools, including the 2016 National School on Neutron and X-Ray Scattering, the 2017 US School on Total Scattering Analysis, the 2017 Modern Methods in Rietveld Refinement for Structural Analysis School, and the 2017 National School on Neutron and X-Ray Scattering.

Los Alamos National Laboratory

**Neutron School Instructor** **2014-2015**

Taught the hands on portion of the small angle scattering section of the school. Theme of the 2014 school was “Geosciences and Materials in Extreme Environments”. Also taught the small angle portion of the 2015 school with a focus on “Materials at the Mesoscale”.

Michigan State University

**Teaching Assistant** **2007-2012**

Aided in teaching an international course in computational physics in conjunction with TUDelft in the Netherlands. Course emphasis was on developing Fortran and C code for projects involving Monte Carlo, MD, DFT, finite element, etc.

**Journal Club Organizer** **2008**

Organized and hosted a series of lunch time student lectures on a variety of topics in photovoltaic research. This was part of the boot-strapping effort I engaged in to develop a research thrust at MSU to work on organic photovoltaic devices, which continues to this day.

**Teaching Assistant** **2005-2006**

Teaching assistant for the Lyman Briggs college at MSU. Course focused on introductory physics. Work involved lectures, grading, and assisting with homework questions.

ADDITIONAL EXPERIENCE AND OUTREACH

**Basic Energy Science (BES) Highlights Committee Member** **2017-2018**
Diffraction group representative, developing science highlights which were presented bimonthly to funding sponsor (DOE-BES).

**LDRD Experience** **2016-2018**
Led the primary conception and authorship of a successfully funded Laboratory Directed Research and Development (LDRD) proposal, *"Taking $N^2$ to N: Developing a Highly Efficient, Multiscale Modeling Framework for Hierarchical Materials"* (LDRD Project ID 8420).

**Contributed to capture efforts for both Second Target Station and DISCOVER Beamline** **2017**
Active participant in development of science cases for the second target station, specifically a Joint Acquisition of Chemistry and Kinetic Structure (JACKS) beamline concept (combined small, wide, and spectroscopy). Active participant in development of science cases for the upcoming neutron total scattering beamline, DISCOVER, specifically the sample environment concepts and moderator/instrument resolution simulations in regards to optimal PDF measurements.

**Contributed to ACA Outreach Program: Uniqueness and You** **2017**
Helped author the successfully funded ACA Outreach Grant, *"Uniqueness and You: How the Disorder of Atomic Structures Enables Your World"*. Help develop associated curriculum and software tools to educate middle school –and-up aged kids about the wonders of diffraction. See some of this work at www.myatomicstructureworld.org/

**Active Role in Neutron Science Outreach Trailer Development and Presentations** **2017**
Selected to visit local career fairs and US Science & Engineering Festival in Washington, DC, performing outreach activities with Neutron Science Division. Have taken an active role in the development of interactive curriculum materials and the design of a planned upgrade to the Science Fair Trailer program - sciencefair.ornl.gov/

**Participated in National Adopt-a-Physicist Program** **2017**
Engaged with local and national high-school students about what it means to be a scientist at a national laboratory. Advised students on education and career options.

REFERENCES

Dr. Katharine Page – Diffraction Beamline Scientist, Oak Ridge National Laboratory – pagekl@ornl.gov

Dr. Matthew Tucker- Diffraction Group Leader, Oak Ridge National Laboratory – tuckermg@ornl.gov

Dr. Thomas Proffen, Director of the Science Initiative for High Performance Computing and Data Analysis, Oak Ridge National Laboratory – tproffen@ornl.gov

Dr. Phillip Duxbury, Department Chair of Physics and Astronomy, Michigan State University – duxbury@pa.msu.edu

Dr. Rex Hjelm, LQD Beamline Scientist (retired), Los Alamos National Laboratory – rexhjelm@icloud.com

Dr. Claire White, Assistant Professor of Civil & Environmental Engineering, Princeton University – whitece@Princeton.edu

Dr. James R. Neilson, Assistant Professor of Chemistry, Colorado State University – james.neilson@colostate.edu