



## PANDA Citation Listing Report

All approved publications with the following search criteria

Report Preparer: Toby, Brian H.

Author Id: Gursoy, Doga (#232951)

---

Bhimji, Wahid, Debbie Bard, Melissa Romanus, David Paul, Andrey Ovsyannikov, Brian Friesen, Matt Bryson, "Accelerating Science with the NERSC Burst Buffer Early User Program." Paper presented at the 2016 Cray User Group: Scalability, London GB, May 8, 2016 - May 12, 2016.

Bicer, Tekin, Doga Gursoy, Rajkumar Kettimuthu, Francesco De Carlo, Ian Foster. "Optimization of Tomographic Reconstruction Workflows on Geographically Distributed Resources." *Journal of Synchrotron Radiation* 23 Jul, 2016: 997-1005. doi: 10.1107/S1600577516007980.

Bicer, Tekin, Doga Gursoy, Rajkumar Kettimuthu, Francesco De Carlo, Gagan Agrawal, Ian Foster. "Rapid Tomographic Image Reconstruction via Large-Scale Parallelization." Paper presented at the 2015 Euro Par, Vienna AT, August 24, 2015 - August 28, 2015. Published in *Lecture Notes in Computer Science*, : 289-302. Springer, 2015.

Chen, Yujia, Kun Wang, Doga Gursoy, Carmen Hoyuelos, Francesco De Carlo, Mark Anastasio. "Joint Reconstruction of Absorption and Refractive Properties in Propagation-Based X-ray Phase-Contrast Tomography via a Non-Linear Image Reconstruction Algorithm." Paper presented at the 2016 SPIE Medical Imaging Conference, San Diego, CA US, February 27, 2016 - March 3, 2016.

Ching, Daniel, Doga Gursoy. "Xdesign: An open-source software package for designing X-ray imaging phantoms and experiments." *Journal of Synchrotron Radiation* (forthcoming).

De Andrade, Vincent, Alex Deriy, Michael Wojcik, Doga Gursoy, Deming Shu, Tim Mooney, Kevin Peterson, "A New Transmission X-ray Microscope for In-Situ Nano-Tomography at the Advanced Photon Source." Abstract of paper presented at the 2016 Developments in X Ray Tomography X, San Diego, CA US, August 28, 2016 - September 1, 2016.

De Carlo, Francesco, Doga Gursoy, F Marone, M Rivers, D Parkinson, Faisal Khan, Nicholas Schwarz, "Scientific Data Exchange: A Schema for HDF5-Based Storage of Raw and Analyzed Data." *Journal of Synchrotron Radiation* (forthcoming).

De Carlo, Francesco, Doga Gursoy, F Marone, M Rivers, D Parkinson, Faisal Khan, Nicholas Schwarz, "Scientific Data Exchange: a Schema for HDF5-Based Storage of Raw and Analyzed Data." *Journal of Synchrotron Radiation* 21 2014: 1224-1230. doi: 10.1107/S160057751401604X.

Duke, Daniel, Andrew Swantek, N. Sovis, F. Tilocco, A. Kastengren, Doga Gursoy, Tekin Bicer, et al. *X-ray Tomography of Multi-hole Gasoline Direct Injectors*. URL, 5:30. (forthcoming). <https://www.dropbox.com/s/sz8t3npzniwk7qb/GDI%20Tomography%201080p.avi?dl=0>.

Duke, Daniel, Andrew Swantek, Nicholas Sovis, F. Tilocco, Alan Kastengren, Doga Gursoy, Christopher Powell. "Time-resolved X-ray Tomography of Gasoline Direct Injection Sprays." Paper presented at the 2015 Powertrains, Fuels and Lubricants, International Meeting, Kyoto JP, September 1, 2015 - September 4, 2015.

Dyer, Eva, William Roncal, Hugo Fernandes, Doga Gursoy, Xianghui Xiao, Joshua Vogelstein, Chris Jacobsen, et al. "Quantifying mesoscale neuroanatomy using X-ray microtomography." *Nature Methods* (forthcoming).

---

Gursoy, Doga, Francesco De Carlo, Xianghui Xiao, Chris Jacobsen. "TomoPy: A framework for the Analysis of Synchrotron Tomographic Data." *Journal of Synchrotron Radiation* 21, no. 5 Sep 1, 2014: 1188-1193. doi: 10.1107/S1600577514013939.

Gursoy, Doga, Francesco De Carlo, Xianghui Xiao, Chris Jacobsen. "TomoPy: A Framework for the Analysis of Synchrotron Tomographic Data." Paper presented at the LEGACY DEFAULT CONFERENCE, San Diego, CA, January 1, 1900 - October 1, 2014.

Gursoy, Doga, Francesco De Carlo, Xianghui Xiao, Christopher Jacobsen. "TomoPy: A Framework for the Analysis of Synchrotron Tomographic Data." *Journal of Synchrotron Radiation* 21, no. 5 Aug 1, 2014: 1188-1193. doi: 10.1107/S1600577514013939.

Gursoy, Doga, Shane Sullivan, Stefan Vogt. "Evaluation of Contemporary Data Acquisition Schemes for X-ray Fluorescence Tomography." Abstract of paper presented at the 65th Annual Conference on Applications of X-ray Analysis, Chicago, IL US, August 1, 2016 - August 5, 2016.

Gürsoy, Do a, Tekin Bicer, Jonathan Almer, Rajkumar Kettimuthu, Stuart Stock, Francesco De Carlo. "Maximum a posteriori estimation of crystallographic phases in X-ray diffraction tomography." *Philosophical Transactions of the Royal Society A: Mathematical, Physical & Engineering Sciences* 373, no. 2043 Jun 13, 2015 doi: 10.1098/rsta.2014.0392.

Gürsoy, Do a, Tekin Bicer, Antonio Lanzirotti, Matthew Newville, Francesco De Carlo. "Hyperspectral Image Reconstruction for X-ray Fluorescence Tomography." *Optics Express* 23, no. 7 Apr 7, 2015: 9014-9023. doi: 10.1364/OE.23.009014.

O'Brien, Sarah, Matthew Whiteside, Deirdre Sholto-Douglas, Alice Dohnalkova, Daniel Durall, Gursoy Doga, Melanie Jones, "Identifying microbial habitats in soil using quantum dots and x-ray fluorescence microtomography." Poster presented at the 7th Annual Argonne Soil Metagenomics Meeting, Lisle, IL US, October 21, 2015-October 23, 2015.

Pelt, Daniël, Doğa Gürsoy, Willem Palenstijn, Jan Sijbers, Francesco De Carlo, Kees Batenburg. "Integration of TomoPy and the ASTRA toolbox for advanced processing and reconstruction of tomographic synchrotron data." *Journal of Synchrotron Radiation* 23 May, 2016: 842-849. doi: 10.1107/S1600577516005658.

Phatak, C. , D. Gursoy. "Iterative Reconstruction of Magnetic Induction using Lorentz Transmission Electron Tomography." *Ultramicroscopy* 150 Mar, 2015: 54-64. doi: 10.1016/j.ultramic.2014.11.033.

Phatak, C. , D Gursoy, E Gulsoy, L Trahey, V De Andrade. "Integrated Multimodal Imaging of Cathodes for Lithium Ion Battery." Abstract of paper presented at the 145th TMS Annual Meeting and Exhibition , Nashville, TN US, February 14, 2016 - February 18, 2016.

Phatak, C. , X. Yang, D. Gursoy, L Trahey, E. Gulsoy, V. De Andrade, X. Xiao, et al."Integrated Multimodal Imaging: From Functional Nanostructures to Lithium Ion Battery Cathodes." Slide presentation at the 25th International Materials Research Congress, Cancun MX, August 14, 2016 - August 19, 2016.

Phatak, C. , X Yang, D Gursoy, E Gulsoy, L Trahey, V De Andrade, Q Liu, et al."MIMES: Multimodal Imaging of Materials for Energy Storage." Slide presentation at the 145th TMS Annual Meeting and Exhibition , Nashville, TN US, February 14, 2016 - February 18, 2016.

Roncal, William, Eva Dyer, Doga Gürsoy, Konrad Kording, Narayanan Kasthuri. "From sample to knowledge: Towards an integrated approach for neuroscience discovery." *Frontiers in Synaptic Neuroscience* (forthcoming).

Toby, Brian, Do a Gürsoy, Francesco De Carlo, Nicholas Schwarz, Hemant Sharma, Chris Jacobsen. "Practices and standards for data and processing at APS." *Synchrotron Radiation News* 28, no. 2 Mar, 2015: 15-20. doi: 10.1080/08940886.2015.1013415.

Yang, X., D. Gursoy, C. Phatak, V. De Andrade, E. Gulsoy, F. De Carlo. "Learning from Scanning Transmission Electron Microscopy to Enhance Transmission X-ray Microscopy: How we can merge STEM and TXM datasets?." Abstract of paper presented at the 2016 Microscopy and Microanalysis Meeting, Columbus, OH US, July 24, 2016 - July 28, 2016.

Yang, Xiaogang, Doga Gursoy, Charudatta Phatak, Vincent De Andrade, E. Gulsoy, Francesco De Carlo. "Enhancing structural resolution of Lithium-ion battery particles by multimodal analysis of TXM and STEM datasets." Slide presentation at the 3rd International Congress on 3D Materials Science, St. Charles, IL US, July 10, 2016 - July 13, 2016.



## PANDA Citation Listing Report

All approved publications with the following search criteria

Report Preparer: Toby, Brian H.  
Author Id: Bicer, Tekin (#240474)

---

Bicer, Tekin, Doga Gürsoy, Rajkumar Kettimuthu, Francesco De Carlo and Ian Foster. "Optimization of Tomographic Reconstruction Workflows on Geographically Distributed Resources." *Journal of Synchrotron Radiation* 23 Jul, 2016: 997-1005. doi: 10.1107/S1600577516007980.

Bicer, Tekin, Do a Gürsoy, Rajkumar Kettimuthu, Francesco De Carlo, Gagan Agrawal and Ian Foster. "Rapid Tomographic Image Reconstruction via Large-Scale Parallelization." Paper presented at the 2015 Euro Par, Vienna AT, August 24, 2015 - August 28, 2015. Published in *Lecture Notes in Computer Science*, : 289-302. Springer, 2015.

Duke, Daniel, Andrew Swantek, N. Sovis, F. Tilocco, A. Kastengren, Doga Gürsoy, Tekin Bicer and et al. *X-ray Tomography of Multi-hole Gasoline Direct Injectors*. URL, 5:30. (forthcoming). <https://www.dropbox.com/s/sz8t3npzniwk7qb/GDI%20Tomography%201080p.avi?dl=0>.

Gürsoy, Do a, Tekin Bicer, Jonathan Almer, Rajkumar Kettimuthu, Stuart Stock and Francesco De Carlo. "Maximum a posteriori estimation of crystallographic phases in X-ray diffraction tomography." *Philosophical Transactions of the Royal Society A: Mathematical, Physical & Engineering Sciences* 373, no. 2043 Jun 13, 2015 doi: 10.1098/rsta.2014.0392.

Gürsoy, Do a, Tekin Bicer, Antonio Lanzirotti, Matthew Newville and Francesco De Carlo. "Hyperspectral Image Reconstruction for X-ray Fluorescence Tomography." *Optics Express* 23, no. 7 Apr 7, 2015: 9014-9023. doi: 10.1364/OE.23.009014.



## PANDA Citation Listing Report

**All approved publications with the following search criteria**

Report Preparer: Toby, Brian H.

Author Id: Di, Zichao (#231822)

---

Di, Zichao, Si Chen, Young Pyo Hong, Chris Jacobsen, Sven Leyffer and Stefan Wild. "Joint Reconstruction of X-Ray Fluorescence and Transmission Tomography." *Optics Express* (forthcoming).

Di, Zichao, Sven Leyffer and Stefan Wild. "Optimization-Based Approach for Joint X-ray Fluorescence and Transmission Tomographic Inversion." *SIAM Journal on Imaging Sciences* 9, no. 1 2016: 1-23. doi: 10.1137/15M1021404 .

Lin, Fu, Zichao Di and Sven Leyffer. "A Multiscale Approach to A Class of Semidefinite Programs." Paper presented at the American Control Conference, null, null.



## PANDA Citation Listing Report

All approved publications with the following search criteria

Report Preparer: Toby, Brian H.

Author Id: Sharma, Hemant (#229389)

---

Naragani, Diwakar, M.D. Sangid, Paul Shade, Jay Schuren, Jun-Sang Park, Peter Kenesei, Hemant Sharma, et al. "Investigation of fatigue crack initiation from a non-metallic inclusion via high energy x-ray diffraction microscopy ." *Acta Materialia* (forthcoming).

Paranjape, Harshad, Paul P. Partha, Hemant Sharma, Peter Kenesei, Jun-Sang Park, T. W. Duerig, Aaron Stebner and et al. "Influences of Granular Constraints and Surface Effects on the Heterogeneity of Elastic, Superelastic, and Plastic Responses of Polycrystalline Shape Memory Alloys ." *Journal of the Mechanics and Physics of Solids* (forthcoming).

Park, Jun-Sang, Peter Kenesei, Hemant Sharma, Ali Mashayekhi, John Okasinski, Jonathan Almer, Erika Benda, "High-energy x-ray techniques for studying nuclear energy relevant materials." Poster presented at the 2015 APS/CNM Users Meeting, Argonne, IL US, May 11, 2015-May 14, 2015.

Park, Jun-Sang, Xuan Zhang, Hemant Sharma, David Hoelzer, Meimei Li, Jonathan Almer. "High-Energy Synchrotron X-ray Techniques for Studying Irradiated Materials." *Journal of Materials Research* 30, no. 9 May 14, 2015: 1380-1380. doi: 10.1557/jmr.2015.50.

Sharma, H., J. Sietsma, S.E. Offerman. "Preferential Nucleation during Polymorphic Transformations." *Scientific Reports* 6 Aug 3, 2016 doi: 10.1038/srep30860.

Toby, Brian, Do a Gürsoy, Francesco De Carlo, Nicholas Schwarz, Hemant Sharma, Chris Jacobsen. "Practices and standards for data and processing at APS." *Synchrotron Radiation News* 28, no. 2 Mar, 2015: 15-20. doi: 10.1080/08940886.2015.1013415.

Wozniak, Justin, Hemant Sharma, Timothy G. Armstrong, Michael Wilde, Jonathan Almer, Ian Foster. "Big Data Staging with MPI-IO for Interactive X-ray Science." Paper presented at the 2014 IEEE/ACM International Symposium on Big Data Computing ,7th IEEE/ACM International Conference on Utility and Cloud Computing, London GB, December 8, 2014 - December 11, 2014.

Zhang, Xuan, Jun-Sang Park, Chi Xu, Hemant Sharma, Jonathan Almer, Meimei Li. "3D Study of Deformation Behavior in Neutron Irradiated Fe-9Cr Alloy." Slide presentation at the 65th Annual Conference on Applications of X-ray Analysis, Chicago, IL US, August 1, 2016 - August 5, 2016. Published in *High-Energy X-ray Microscopy*, (forthcoming).

Zhang, Xuan, Chi Xu, Meimei Li, Jun-Sang Park, Peter Kenesei, Hemant Sharma, Jonathan Almer. "In-situ and 3D X-ray Diffraction Study of Deformation Behavior in Neutron-Irradiated Fe-9%Cr Polycrystal." Slide presentation at the 2016 Nuclear Fuels & Structural Materials Topical Meeting held at 2016 American Nuclear Society Annual Meeting, New Orleans, LA US, June 12, 2016 - June 16, 2016.

Zhang, Xuan, Chi Xu, Jun-Sang Park, Hemant Sharma, Peter Kenesei, Jonathan Almer, Meimei Li. "3D Study of Neutron Irradiation Effects on Tensile Deformation in Fe-based Alloys using High Energy Synchrotron X-rays ." Abstract of paper presented at the ANS Annual Meeting, Embedded Topical Meeting: Nuclear Fuels and Structural Materials for the Next Generation Nuclear Reactors, Reno, NV, June 4, 2006 - June 8, 2006.



## PANDA Citation Listing Report

All approved publications with the following search criteria

Report Preparer: Toby, Brian H.

Author Id: Toby, Brian (#56929)

---

Antao, Sytle, I Hassan, W Mulder, Peter Lee and Brian Toby. "In situ study of the  $R\bar{3}c$ - $R\bar{3}m$  orientational disorder in calcite." *Physics and Chemistry of Minerals* 36 2009: 159-169. doi: 10.1007/s00269-008-0266-y.

Ayer, Vidya, Sheila Miguez and Brian Toby. "Why Scientists Should Learn to Program in Python." *Powder Diffraction* 29, no. S2 Dec, 2014: S48-S64. doi: 10.1017/S0885715614000931.

Cui, Jun, Q Huang and Brian Toby. "Magnetic structure refinement with neutron powder diffraction data using GSAS : a tutorial." *Powder Diffraction* 21, no. 1 Mar, 2006: 71-79. doi: 10.1154/1.2179805.

Cui, Jun, Q Huang and Brian Toby. "Magnetic structure refinement with neutron powder diffraction data using GSAS : a tutorial." *Powder Diffraction* 21, no. 1 2006: 71-79. .

DeSanto Jr., P, D Buttrey, R Grasselli, W Pyrz, C Lugmair, A Volpe Jr., T Vogt and et al."Comparision of MoVTaTeO and MoVNBTeO M1 crystal chemistry." *Topics in Catalysis* 38, no. 1-3 2006: 31-40. doi: 10.1007/s11244-006-0068-8.

DeSanto Jr., P, D Buttrey, R Grasselli, W Pyrz, C Lugmair, A Volpe Jr., T Vogt and et al."Comparison oof MoVTaTeO and MoVNBTeO M1 crystal chemistry." *Topics in Catalysis* 38, no. 1-3 Jul, 2006: 31-40. .

Egami, Takeshi, Brian Toby, Simon Billinge, James Jorgensen, H Rosenfeld, David Hinks, Bogdan Dabrowski, "Local structural anomaly near  $T\sub c$  observed by pulsed neutron." Paper presented at the 3rd International Conference on Materials and Mechanisms of Superconductivity High-Temperature Superconductors, Kanazawa, Japan, July 22, 1991 - July 26, 1991.

Evans, K, Francesco De Carlo, Pete Jemian, Jonathan Lang, Ulrich Lienert, John Maclean, Matthew Newville, et al."2006 XSD Scientific Software Workshop report."Argonne National Laboratory, ANL/APS/TB-51, .

Fernandez, Patricia, Lahsen Assoufid, Nino Miceli, Deming Shu, Brian Toby, Nicholas Schwarz. "Optics, Detectors, Data, and Instrumentation Engineering at the Advanced Photon Source." Slide presentation at the 5th Diffraction Limited Storage Ring (DLSR) Workshop, Hamburg DE, March 9, 2016 - March 11, 2016.

Fernandez-Rodriguez, Javier, Brian Toby, Michel van Veenendaal. "Mixed configuration ground state in iron(II) phthalocyanine." *Physical Review B: Condensed Matter and Materials Physics* 91, no. 21 Jun 23, 2015 doi: 10.1103/PhysRevB.91.214427.

Jain, P, N Dala, Brian Toby, H Kroto, A Cheetham. "Order-disorder antiferroelectric phase transition in a hybrid inorganic-organic framework with the perovskite architecture." *Journal of the American Chemical Society* 130, no. 32 Aug 13, 2008: 10450-10451. doi: 10.1021/ja801952e.

Jain, P, V Ramachandran , R Clark, Hua Zhou, Brian Toby, N Dalal, H Kroto, et al."Multiferroic behavior associated with an order-disorder hydrogen bonding transition in metal-organic frameworks (MOFs) with the perovskite  $ABX\sub 3$  arhitecture." *Journal of the American Chemical Society* 131, no. 38 Sep 30, 2009: 13625-13627. doi: 10.1021/ja904156s.

---

Jia, S, P Jiramongkolchai, Matthew Suchomel, Brian Toby, J Checkelsky, N Ong, Robert Cava. "Ferromagnetic quantum critical point induced by dimer-breaking in  $\text{SrCo}_{2}(\text{Ge}_{1-x}\text{P}_{x})_{2}$ ." *Nature Physics* 7 2011: 207-210. doi: 10.1038/nphys1868.

Kodama, Richard, M Vedpathak, J Borchers, Brian Toby, S Makhlof. "Evidence for multi-sublattice spin states in NiO nanoparticles." *Applied Physics Letters* (forthcoming).

Lake, C, Brian Toby. "Rigid body refinements in GSAS / EXPGUI." *Powder Diffraction* 26, no. S1 2011: S13-S21. doi: 10.1154/1.3661125.

Lake, C, Brian Toby. "Recent developments targeting new and experienced users in EXPGUI, an open source Rietveld analysis interface." *Zeitschrift für Kristallographie* 226, no. 12 Dec, 2011: 892-897. doi: 10.1524/zkri.2011.1378.

Lee, Peter, Deming Shu, M Ramanathan, Curt Preissner, J Wang, Mark Beno, R VonDreele, "A twelve-analyzer detector system for high-resolution powder diffraction." *Journal of Synchrotron Radiation* 15, no. 5 2008: 427-432. doi: 10.1107/S0909049508018438.

Leighton, Christopher, Jie Wu, D Stauffer, Jeffrey Lynn, Brian Toby, Q Huang, John Mitchell. "Anisotropy-driven magnetic anomalies in  $\text{Pr}_{1-x}\text{Sr}_{x}\text{CoO}_{3}$ ." Paper presented at the 2006 March Meeting of the American Physical Society, Baltimore, MD, March 13, 2006 - March 17, 2006.

Li, D, B O'Connor, It-M Low, A Riessen, Brian Toby. "Mineralogy of Al-substituted goethites." *Powder Diffraction* (forthcoming).

Lobanov, Maxim, Elad Caspi, M Greenblatt, James Jorgensen, Brian Toby, Peter Stephens, D Sheptyakov, et al. "Crystal and magnetic structure of the  $\text{Ca}_{3}\text{Mn}_{2}\text{O}_{7}$  Ruddlesden-Popper phase : neutron and synchrotron x-ray diffraction study." *Journal of Physics : Condensed Matter* 16, no. 29 Jul 28, 2004: 5339-348. doi: 10.1088/0953-8984/16/29/023.

Madden, Timothy, Robert Von Dreele, Brian Toby, Jonathan Baldwin, Matthew Suchomel. "Scanning CCD for X-ray Powder Diffraction." Paper presented at the SRI 2013, Gaithersburg, MD, June 19, 2013 - June 21, 2013.

Madden, Timothy, Robert Von Dreele, Brian Toby, Matthew Suchomel, Jonathan Baldwin, John Weizeorick. "Scanning high resolution CCD detector for powder diffraction." Paper presented at the APS User Meeting, Argonne, IL, May 7, 2012 - May 10, 2012.

Papoular, R, Brian Toby, V Davydov, A Rakhmanina, A Dzyabchenko, H Allouchi, V Agafonov. "Single-crystal and synchrotron x-ray powder diffraction study of the one-dimensional orthorhombic polymer phase of  $\text{C}_{60}$ ." *Chemical Physics Letters* 460, no. 1-3 Jul 20, 2008: 93-99. .

Preissner, Curt, Deming Shu, Peter Lee, Brian Toby, David Kline, Kurt Goetze. "The sample changing robot for the 11-BM high-throughput powder diffraction beamline." Paper presented at the Synchrotron Radiation Instrumentation (SRI2007), Baton Rouge, LA, April 25, 2007 - April 27, 2007.

Preissner, Curt, Deming Shu, Peter Lee, Brian Toby, J Wang, David Kline, Kurt Goetze. "The sample-changing robot for the 11-BM high-throughput powder diffraction beamline." Poster presented at the MEDSI/SRI 2008, Saskatchewan, Canada, June 10, 2008-June 13, 2008.



Preissner, Curt, Deming Shu, Peter Lee, Brian Toby, J Wang, David Kline, Kurt Goetze. "The sample-changing robot for the 11-BM high-throughput powder diffraction beamline." Paper presented at the MEDSI/SRI 2008, Saskatchewan, Canada, June 10, 2008 - June 13, 2008.

Preissner, Curt, Deming Shu, Brian Toby, P Lee, J Wang, David Kline, Kurt Goetze. "The sample-changing robot for the 11-BM high-throughput powder diffraction beamline." Paper presented at the MEDSI/SRI 2008, Saskatchewan, Canada, June 10, 2008 - June 13, 2008.

Ribaud, Lynn, Charles Kurtz, Brian Toby. "Inexpensive in-vacuum connectors for wiring harnesses." *Review of Scientific Instruments* (forthcoming).

Shu, Deming, Peter Lee, Curt Preissner, M Ramanathan, Mark Beno, R VonDreele, R Raney, "Mechanical design of a high-resolution x-ray powder diffractometer at the Advanced Photon Source." Paper presented at the Society of Photo-Optical Instrumentation Optics + Photonics Conference, San Diego, CA, August 26, 2007 - August 30, 2007.pp. 6665ON.

Shu, Deming, Peter Lee, Curt Preissner, M Ramanathan, Mark Beno, Robert Von Dreele, R Raney, "Mechanical design of a high-resolution x-ray powder diffractometer at the Advanced Photon Source." Paper presented at the SPIE Optics and Photonics 2007, San Diego, CA, August 26, 2007 - August 30, 2007.

Shu, Deming, Peter Lee, M Ramanathan, Mark Beno, Robert Von Dreele, R Raney, Lynn Ribaud, "Mechanical design of a high-resolution x-ray powder diffractometer at the Advanced Photon Source." Paper presented at the SPIE Optics and Photonics 2007, San Diego, CA, August 26, 2007 - August 30, 2007.

Tiley, J, R Srinivasan, R Banerjee, G Viswanathan, Brian Toby, H Fraser. "Application of x-ray and neutron diffraction to determine lattice parameters and precipitate volume fractions in low misfit nickel base superalloys." *Materials Science and Technology* 25, no. 11 2009: 1369-1774. doi: 10.1179/174328409X399010.

Toby, Brian. "Powder Diffraction Crystallography : 98 Years as Plan B?." *LEGACY DEFAULT JOURNAL* (forthcoming).

Toby, Brian. "Observations on online educational materials for powder diffraction crystallography software." *Journal of Applied Crystallography* 43, no. Pt.5 No.2 Oct, 2010: 1271-1275. doi: 10.1107/S0021889810034382.

Toby, Brian. "R-factors in Rietveld : how good is good enough?." *Powder Diffraction* 21, no. 1 2006: 67-70. .

Toby, Brian. "Powder diffraction crystallography software : the present and future." Slide presentation at the 2006 XSD Scientific Software Workshop, Argonne, IL, August 29, 2006.

Toby, Brian. "Computer Software, Powder Diffraction and Science." Dec, 2014.

Toby, Brian. "A new approach for instruction in powder crystallography." *Powder Diffraction* 22, no. 1 Mar, 2007: 83-84. .

Toby, Brian. "Rietveld Refinement." (forthcoming).

Toby, Brian, Bachir Aoun, Eric Pellegrini, Marcus Trapp, Francesca Natali, Laura Cantù, Paola Brocca, "Direct comparison of elastic incoherent neutron scattering experiments with molecular dynamics simulations of DMPC phase transitions." *The European Physical Journal E: Soft Matter* 39, no. 48 2016 doi: 10.1140/epje/i2016-16048-y.

Toby, Brian, Do a Gürsoy, Francesco De Carlo, Nicholas Schwarz, Hemant Sharma, Chris Jacobsen. "Practices and standards for data and processing at APS." *Synchrotron Radiation News* 28, no. 2 Mar, 2015: 15-20. doi: 10.1080/08940886.2015.1013415.

Toby, Brian, Yu Huang, Donald Dohan, D Carroll, Xuesong Jiao, Lynn Ribaud, J Doebbler, "Management of metadata and automation for mail-in measurements with the APS 11-BM high throughput, high-resolution synchrotron powder diffractometer." *Journal of Applied Crystallography* 42 Dec, 2009: 990-993 (Pt. 6). doi: 10.1107/S0021889809035717.

Toby, Brian, C Lind. "Powder diffraction crystallography resources." *Powder Diffraction Crystallography Resources*. [http://www.aps.anl.gov/Xray\\_Science\\_Division/Powder\\_Diffraction\\_Crystallography/](http://www.aps.anl.gov/Xray_Science_Division/Powder_Diffraction_Crystallography/).

Toby, Brian, Timothy Madden, Matthew Suchomel, Jonathan Baldwin, Robert Von Dreele. "A Scanning CCD Detector for Powder Diffraction Measurements." *Journal of Applied Crystallography* (forthcoming).

Toby, Brian, Robert Von Dreele. "GSAS-II: the genesis of a modern open-source all-purpose crystallography software package." *Journal of Applied Crystallography* (forthcoming).

Toby, Brian, Robert Von Dreele. "What's New in GSAS-II." *Powder Diffraction* 29, no. S2 Dec, 2014: S2-S6. doi: 10.1017/S0885715614000736.

Varga, Tamas, John Mitchell, Brian Toby, J Wang, Christos Malliakas, L Arnold. "High-pressure synthesis, crystal and electronic structures of a new scandium tungstate,  $\text{Sc}_{0.67}\text{WO}_4$ ." *Journal of Solid State Chemistry* 183, no. 7 2010: 1567-1573. doi: 10.1016/j.jssc.2010.04.039.

Von Dreele, Robert, Brian Toby. "X-ray powder diffraction." (forthcoming).

Wang, J, Brian Toby, Peter Lee, Lynn Ribaud, Sytle Antao, Charles Kurtz, M Ramanathan, et al. "A dedicated powder diffracton beamline at the Advanced Photon Source : Commissioning and early operational results." *Review of Scientific Instruments* 79 2008: 08515. doi: 10.1063/1.2969260.



## PANDA Citation Listing Report

All approved publications with the following search criteria

Report Preparer: Toby, Brian H.

Author Id: Van Veenendaal, Michel (#50671)

---

Ahn, K, Arthur Fedro and Michel Van Veenendaal. "Dynamics and spectral weights of shake-up valence excitations in resonant inelastic x-ray scattering." *Physical Review Letters* (forthcoming).

Casa, Diego, J Kim, Mary Upton, Thomas Gog, Yong-Tae Kim, Michel Van Veenendaal, Jeroen van den Brink, "Entangled spin-orbital waves in Sr<sub>2</sub>IrO<sub>4</sub> observed by resonant inelastic x-ray scattering." *Science* (forthcoming).

Casa, Diego, J Kim, Mary Upton, Thomas Gog, Michel Van Veenendaal, Jeroen van den Brink, Y-J Kim, "Magnetic excitation spectra of Sr<sub>2</sub>IrO<sub>4</sub> probed by resonant inelastic x-ray scattering: establishing links to cuprate superconductivity." *Physical Review Letters* 108, no. 17 2012: 177003. doi: 10.1103/PhysRevLett.108.177003.

Casa, Diego, J Kim, Mary Upton, Thomas Gog, Michel Van Veenendaal, Jeroen van den Brink, Y-J Kim, "Isospin dynamics in Sr<sub>2-x</sub>IrO<sub>4-x</sub>: forging links to cuprate superconductivity." *Physical Review Letters* (forthcoming).

Chakhalian, J, John Freeland, H Habermeier, G Cristiani, G Khaliullin, Michel Van Veenendaal, B Keimer. "Orbital reconstruction and covalent bonding at an oxide interface." *Science* 318 Nov 16, 2007: 1114-1117. .

Chang, J, Arthur Fedro, Michel Van Veenendaal. "Ultrafast cascading in intersystem crossings in transition-metal complexes." *Physical Review B: Condensed Matter and Materials Physics* 82 Aug 12, 2010: 075124. doi: 10.1103/PhysRevB.82.075124.

Chang, J, Michel Van Veenendaal, Arthur Fedro. "Ultrafast electron dynamics theory of photo-excited ruthenium complexes." *Physical Review Letters* (forthcoming).

Chen, Cheng-Chien, Michel van Veenendaal, Thomas Devereaux, Krzysztof Wohlfeld. "Fractionalization, entanglement, and separation: understanding the collective excitations in a spin-orbital chain." *Physical Review B: Condensed Matter* 91, no. 16 Apr 2, 2015 doi: 10.1103/PhysRevB.91.165102.

Chikara, Shalinee, Daniel Haskel, Kang-Hwan Kim, Heung-Sik Kim, Cheng-Chien Chen, G. Fabbris, L. S. I. Veiga, "Sr<sub>2</sub>Ir<sub>1-x</sub>Rh<sub>x</sub>O<sub>4</sub>: an inhomogeneous  $j_{\text{eff}} = 1/2$  Hubbard system." *Physical Review Letters* 92, no. 8 Aug 24, 2015 doi: 10.1103/PhysRevB.92.081114 .

Chikara, Shalinee, Daniel Haskel, Jae-Hoon Sim, Cheng-Chien Chen, G. Fabbris, L.S. Veiga, N Souza-Neto, "Sr<sub>2</sub>Ir<sub>1-x</sub>Rh<sub>x</sub>O<sub>4</sub> ( $x < 0.5$ ): an inhomogeneous  $j_{\text{eff}} = 1/2$  Hubbard system." *Physical Review B: Rapid Communications* 92 2015 doi: 10.1103/PhysRevB.92.081114.

Chikara, Shalinee, Daniel Haskel, Jae-Hoon Sim, Heung-Sik Kim, Cheng-Chien Chen, G. Fabbris, L. S. I. Veiga, "Sr<sub>2</sub>Ir<sub>(1-x)</sub>Rh<sub>x</sub>O<sub>4</sub>: an inhomogeneous  $j_{\text{eff}} = 1/2$  Hubbard system." *Physical Review Letters* 92, no. 8 Aug 24, 2015 doi: 10.1103/PhysRevB.92.081114 .

Ding, Yang, Cheng-Chien Chen, Heung-Sik Kim, Myung Han, Zhenxing Feng, Mary Upton, Jungho Kim, "Elementary Excitations in High-Pressure Resonant Inelastic X-ray Scattering Measurement of Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub>." *Physical Review Letters* (forthcoming).

Ding, Yang, Cheng-Chien Chen, Q Zeng, H Kim, M Han, Mahalingam Balasubramanian, R Gordon, "A Novel High-Pressure Monoclinic Metallic Phase of V<sub>2</sub>O<sub>3</sub>." *Physical Review Letters* (forthcoming).

Ding, Yang, Javier Fernandez-Rodriguez, J Kim, F Li, Diego Casa, Mary Upton, Thomas Gog, et al. "Spin-Ordering Mediated Orbital Hybridization in CoO at High Pressure." *Physical Review Letters* 86, no. 9 Sep, 2012: 094107. doi: 10.1103/PhysRevB.86.094107.

Ding, Yang, Daniel Haskel, Eiji Kaneshita, Y Tseng, Michel Van Veenendaal, John Mitchell, Stanislav Sinogeikin, et al. "Pressure-induced magnetic transition in manganite (La<sub>0.75</sub>Ca<sub>0.25</sub>MnO<sub>3</sub>)." *Physical Review Letters* 102 2009: 2372011. doi: 10.1103/PhysRevLett.102.237201.

Ding, Yang, Liuxiang Yang, Cheng-Chien Chen, Heung-Sik Kim, Zhenxing Feng, Mary Upton, Diego Casa, et al. "Pressure-Induced Confined Metal from the Mott Insulator Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub>." *Physical Review Letters* 116, no. 21 May 24, 2016 doi: 10.1103/PhysRevLett.116.216402.

Erdin, Serkan, Michel Van Veenendaal. "A possible mechanism for photoinduced effects in molecule-based magnets." Paper presented at the 2006 March Meeting of the American Physical Society, Baltimore, MD, March 13, 2006 - March 17, 2006.

Fernandez-Rodriguez, Javier, Brian Toby, Michel van Veenendaal. "Mixed configuration ground state in iron(II) phthalocyanine." *Physical Review B: Condensed Matter and Materials Physics* 91, no. 21 Jun 23, 2015 doi: 10.1103/PhysRevB.91.214427.

Freeland, John, Michel Van Veenendaal, Kenneth Gray, Qing'an Li, Hong Zheng, J Mitchell. "Role of oxygen in the orbital ordered state of La<sub>0.5</sub>Sr<sub>1.5</sub>MnO<sub>4</sub>." Paper presented at the American Physical Society March Meeting, Denver, CO, March 5, 2007 - March 9, 2007.

Freeland, John, Michel van Veenendaal, J Tchakhalian. "Evolution of Electronic Structure Across the Rare-Earth RNiO<sub>3</sub>." *Journal of Electron Spectroscopy and Related Phenomena* 208, no. SI Apr, 2016: 56-62. doi: 10.1016/j.elspec.2015.07.006 .

Han, Myung, J, Michel Van Veenendaal. "Electronic structure and orbital polarization of LaNiO<sub>3</sub> with a reduced coordination and under strain : first-principals study." *Physical Review B: Condensed Matter and Materials Physics* (forthcoming).

Haskel, Daniel, G Fabbris, M Laguna Marco, N Souza-Neto, Michel Van Veenendaal, G Cao. "Electronic ground state properties of Iridate oxides from x-ray absorption spectroscopy." Paper presented at the Kentucky Condensed Matter Physics Symposium: The Iridates, Lexington, KY, April 28, 2012 - April 29, 2012.

Haskel, Daniel, G Fabbris, Maria Laguna-Marco, Jonathan Lang, N Souza-Neto, Michel Van Veenendaal, James Schilling, et al. "Tuning the spin-orbit coupled ground state of iridates with pressure." Paper presented at the APS March Meeting 2012, Balrimore, MD, March 18, 2013 - March 22, 2013.

Haskel, Daniel, G Fabbris, Mikhail Zhernenkov, Jong Woo Kim, J Kim, Bumjoon Kim, Michel Van Veenendaal, et al. "Tuning the Spin-Orbit Coupled Ground State of Iridates With Pressure." Paper presented at the New opportunities to study magnetism and related phenomenon in 4d & 5d systems, Oak Ridge, TN, July 22, 2013 - July 24, 2013.

Haskel, Daniel, G Fabbris, Mikhail Zhernenkov, P Kong, Changqing Jin, G Cao, Michel Van Veenendaal. "Pressure tuning of the spin-orbit coupled ground state in Sr(sub2)IrO(sub4)." Paper presented at the 12th Joint MMM/Intermag Conference, Chicago, IL, January 14, 2013 - January 18, 2013.

Haskel, Daniel, G Fabbris, Mikhail Zhernenkov, P Kong, Changqing Jin, G Cao, Michel Van Veenendaal. "Pressure tuning of the spin-orbit coupled ground state in Sr(sub2)IrO(sub4)." Paper presented at the MMM Intermag Joint Conference 2013, Chicago, IL, January 14, 2013 - January 18, 2013.

Haskel, Daniel, G Fabbris, Mikhail Zhernenkov, K Panpan, Changqing Jin, G Cao, Michel Van Veenendaal. "Pressure-tuning of spin-orbit coupled ground state in Sr{sub 2}IrO{sub 4}." *Physical Review Letters* (forthcoming).

Haskel, Daniel, Evgeny Kravtsov, A Ankudinov, Jonathan Lang, A Cady, Zahirul Islam, George Srajer, "Dichroic resonant diffraction of circularly polarized x-rays : a route to element-and site-specific magnetism." Paper presented at the 13th International Conference on X-ray Absorption Fine Structure (XAFS 13), Stanford, CA, July 9, 2006 - July 14, 2006.

Haskel, Daniel, Maria Laguna-Marco, N Souza-Neto, Jonathan Lang, G Fabbris, G Cao, Michel Van Veenendaal. "Electronic ground state properties of iridate oxides from x-ray absorption spectroscopy." Paper presented at the APS March Meeting 2012, Boston, MA, February 27, 2012 - March 2, 2012.

Haskel, Daniel, Jonathan Lang, Zahirul Islam, A Cady, George Srajer, Michel Van Veenendaal, P Canfield. "Origin of intrinsic magnetic hardness in permanent magnets." *Physical Review Letters* 95 2005: 217207. .

Haskel, Daniel, Jonathan Lang, Zahirul Islam, A Cady, George Srajer, Michel Van Veenendaal, P Canfield. "Atomic origin of magneto-crystalline anisotropy in Nd(sub 2)Fe(sub 14)B." *Nature* (forthcoming).

Haskel, Daniel, Jonathan Lang, Zahirul Islam, A Cady, George Srajer, Michel Van Veenendaal, P Canfield. "Atomic origin of magneto-crystalline anisotropy in Nd(sub 2)Fe(sub 14)B." *Physical Review Letters* 95, no. 21 2005: 217207. doi: 10.1103/PhysRevLett.95.217207.

Haskel, Daniel, Jonathan Lang, Zahirul Islam, A Cady, George Srajer, Michel Van Veenendaal, P Canfield. "Atomic origin of magneto-crystalline anisotropy in Nd(sub 2)Fe(sub 14)B." *Physical Review Letters* 95 Nov 18, 2005: 217207. doi: 10.1103/PhysRevLett.95.217207.

Haskel, Daniel, Michel Van Veenendaal. "Reply to comment on atomic origin of magneto-crystalline anisotropy in Nd(sub 2)Fe(sub 14)B." *Physical Review Letters* 97 2006: 259702. .

Ito, Yasuo, Michel Van Veenendaal, Russell Cook, N Menon, B Armstrong, D Miller. "Nanometer scale magnetic linear dichroism by EELS." Paper presented at the Microscopy and Microanalysis 2003 (M&M 2003), San Antonio, TX, August 3, 2003 - August 7, 2003.

Janoschek, m. , D. Haskel, J. Fernandez-Rodriguez, M. van Veenendaal, J Rebizant, G. H. Lander, J.-X. Zhu, et al. "The ground state wavefunction of plutonium in PuSb as determined via X-ray Magnetic Circular Dichroism." *Physical Review B: Condensed Matter* 91, no. 3 Jan 14, 2015 doi: 10.1103/PhysRevB.91.035117 .

Laguna-Marco, M., P. Kayser, J. A. Alonso, M. J. Martinez-Lope, M. van Veenendaal, Y. Choi, D. Haskel. "Electronic structure, local magnetism, and spin-orbit effects of Ir(IV)-, Ir(V)-, and Ir(VI)-based compounds." *Physical Review B: Condensed Matter* 91 2015 doi: 10.1103/PhysRevB.91.214433.

Laguna-Marco, Maria, Daniel Haskel, N Souza-Neto, Jonathan Lang, V Krishnamurthy, Shaline Chikara, G Cao, et al. "Orbital magnetism and spin-orbit effects in the electronic structure of BaIrO<sub>3</sub>." *Physical Review Letters* 105, no. 21 Nov 19, 2010: 216407. doi: 10.1103/PhysRevLett.105.216407.

Nemeth, Karoly, Katherine Harkay, Michel Van Veenendaal, Linda Spentzouris, J Terry, M White, Klaus Attenkofer, et al. "Theoretical design of high-brightness photocathodes based on nanostructures." Slide presentation at the Photocathode Physics for Photoinjectors Workshop at Brookhaven National Laboratory, Upton, NY, October 12, 2010 - October 14, 2010.

Nemeth, Karoly, Katherine Harkay, Michel Van Veenendaal, Linda Spentzouris, M White, Klaus Attenkofer, George Srajer. "High-brightness photocathodes through ultrathin surface layers on metals." *Physical Review Letters* 104 Jan 29, 2010: 046801. doi: 10.1103/PhysRevLett.104.046801.

Nemeth, K, K Harkay, Michel Van Veenendaal, L Spentzouris, M White, Klaus Attenkofer, G Srajer . "Theoretical design of high-brightness photocathodes based on ultrathin surface layers on metals and on nanostructures." Paper presented at the 2010 Advanced Accelerator Concepts, Annapolis, MD, June 13, 2010 - June 19, 2010.

Seman, Tsezar, Cheng-Chien Chen, Rajiv Singh, Michel van Veenendaal. "The many faces of quantum kagome materials: Interplay of further-neighbour exchange and Dzyaloshinskii-Moriya interaction." *Physical Review Letters* (forthcoming).

Van Veenendaal, Michel. "Low-energy excitations in the resonant X-ray scattering amplitude." *Physical Review Letters* (forthcoming).

Van Veenendaal, Michel. "Competition between screening channels in core level x-ray photoemission spectroscopy as a probe of changes in ground-state properties of transition-metal compounds." *Physical Review B: Condensed Matter and Materials Physics* 74, no. 8 Aug, 2006: 085118. .

Van Veenendaal, Michel. "L- and m-edge resonant inelastic x-ray scattering in transition-metal compounds." Paper presented at the 5th International Conference on Synchrotron Radiation in Materials Science (SRMS 5), Chicago, IL, July 30, 2006 - August 2, 2006. edited by A. Macrander, et al.

Van Veenendaal, Michel. "Ultrafast insulator-to-metal transitions in vanadium dioxide." *Nature Materials* (forthcoming).

Van Veenendaal, Michel. "Polarization dependence of L- and M-edge resonant inelastic x-ray scattering on transition-metal compounds." *Physical Review Letters* 96, no. 11 Mar 24, 2006: 117404. .

Van Veenendaal, Michel. "3j symbols : to normalize or not to normalize." *The European Physical Journal. Special Topics* 32, no. 4 Jul, 2011: 947-954. doi: 10.1088/0143-0807/32/4/009.

Van Veenendaal, Michel. "Anomalous ground states at the interface of transition-metal compounds." *Physical Review B: Condensed Matter and Materials Physics* 78 2008: 165415. .

Van Veenendaal, Michel, J Chang, Arthur Fedro. "A probability-conserving dissipative Schrodinger equation." *Physical Review Letters* (forthcoming).

Van Veenendaal, Michel, J Chang, Arthur Fedro. "Ultrafast cascading theory of intersystem crossings in transition-metal complexes." *Physical Review B: Condensed Matter and Materials Physics* 82 Aug 12, 2010: 075124. doi: 10.1103/PhysRevB.82.075124.

Van Veenendaal, Michel, Arthur Fedro. "Comment on electron correlation effects in resonant inelastic x-ray scattering of  $\text{NaV}_2\text{O}_5$ ." *Physical Review Letters* 92, no. 21 May, 2004: 219701. doi: 10.1103/PhysRevLett.92.219701.

Van Veenendaal, Michel, M Haverkort. "Effective operator for d-d transitions in nonresonant inelastic x-ray scattering." *Physical Review B: Condensed Matter and Materials Physics* 77 Jun, 2008: 224107. .

Van Veenendaal, Michel, Xin Liu, M Carpenter, S Cramer. "Observation of dd excitations via 4p-3d Coulomb scattering in transition-metal K-edge resonant inelastic scattering." *Physical Review Letters* (forthcoming).

Van Veenendaal, Michel, Ian McNulty. "Prediction of strong dichroism induced by x-rays carrying orbital momentum." *Physical Review Letters* 98 Apr 13, 2007: 157401. .

Veiga, L. S. I., G. Fabbris, M. van Veenendaal, N Souza-Neto, H. Feng, K. Yamaura, D. Haskel. "Fragility of ferromagnetic double exchange interactions and pressure tuning of magnetism in 3d-5d double perovskite  $\text{Sr}_2\text{FeOsO}_6$ ." *Physical Review B: Condensed Matter and Materials Physics* 91, no. 23 Jun 19, 2015 doi: 10.1103/PhysRevB.91.235135.

Wang, Y., B. Moritz, C.-C. Chen, C. Jia, M. van Veenendaal, T. P. Devereaux. "Using Nonequilibrium Dynamics to Probe Competing Orders in a Mott-Peierls System." *Physical Review Letters* 116, no. 8 Feb 24, 2016 doi: 10.1103/PhysRevLett.116.086401.

Wohlfeld, K., Cheng-Chien Chen, M. van Veenendaal, T. Devereaux. "Spin chain in magnetic field: limitations of the large-N mean-field theory." *Acta Physica Polonica A* 127, no. 2 Feb, 2015: 201-203. doi: 10.12693/APhysPolA.127.201.

Yavas, Hasan, Michel Van Veenendaal, Jeroen van den Brink, L Ament, Ahmet Alatas, Bogdan Leu, M Apostu, "Observation of phonons with resonant inelastic x-ray scattering." *Journal of Physics : Condensed Matter* 22, no. 48 2010: 485601. doi: 10.1088/0953-8984/22/48/485601.

van Veenendaal, Michel. "Photoinduced Ultrafast Charge-order Melting: Non-thermal Effects and Charge-order Inversion." *Physical Review B: Condensed Matter and Materials Physics* 94, no. 11 Sep 1, 2016 doi: 10.1103/PhysRevB.94.115101.

van Veenendaal, Michel. "The interaction between X-ray and magnetic vortices." *Physical Review B: Condensed Matter and Materials Physics* 92, no. 24 Dec 10, 2015 doi: 10.1103/PhysRevB.92.245116.



## PANDA Citation Listing Report

All approved publications with the following search criteria

Report Preparer: Toby, Brian H.

Author Id: Von Dreele, Robert (#88348)

---

Avdeev, Maxim, James Jorgensen, Simine Short and Robert Von Dreele. "On the numerical corrections of time-of-flight neutron powder diffraction data." *Journal of Applied Crystallography* 40, no. Pt. 4 2007: 710-715. doi: 10.1107/S0021889807030014.

Cline, J, Robert Von Dreele, R Winburn, Peter Stephens and J Filliben. "Addressing the amorphous content issue in quantitative phase analysis : the certification of NIST SRM 676a." *Acta Crystallographica. Section A: Foundations of Crystallography* 67A, no. 4 Jul, 2011: 357-367. doi: 10.1107/S0108767311014565.

Doebbler, J and Robert Von Dreele. "Macromolecular powder diffraction : structure solution via molecular." Paper presented at the 11th European Powder Diffraction Conference (EPDIC-11), Poland, Warsaw, September 19, 2008 - September 22, 2008.

Doebbler, J and Robert Von Dreele. "Protein structure solution via molecular replacement." Paper presented at the Developments and Directions of Powder Diffractions on Proteins - ESFR, Grenoble, France, June 22, 2007 - June 23, 2007.

Fitzsimmons, Michael, Jeffrey Eastman, Jeffrey Lynn, R Robinson, Robert Von Dreele and Loren Thompson. "Neutron diffraction studies of ultrafine-grain magnetic materials." Paper presented at the Annual Meeting and Exhibition of the Minerals, Metals and Materials Society, Las Vegas, NV, February 12, 1995 - February 16, 1995.

Fitzsimmons, Michael, Jeffrey Eastman, Robert Von Dreele and Loren Thompson. "The roles of grain size and strain on antiferromagnetic order in nanocrystalline chromium." *Physical Review B: Condensed Matter and Materials Physics* 50, no. 8 Aug 15, 1994: 5600-08. .

Harper, J, J Doebbler, E Jaccques, D Grant and Robert Von Dreele. "A combined solid-state NMR and synchrotron x-ray diffraction powder study on the structure of the antioxidant(+)-catechin 4.5 hydrate." *Journal of the American Chemical Society* 132, no. 9 Mar 10, 2010: 2928-2937. doi: 10.1021/ja907671p.

Hunter, Brett, James Jorgensen, John Wagner, Paolo Radaelli, David Hinks, Hagai Shaked, Richard Hitterman and et al. "Pressure-induced structural changes in superconducting  $\text{HgBa}_{2}\text{Ca}_{n-1}\text{Cu}_{n}\text{O}_{2n+2\delta}$  ( $n=1,2,3$ ) compounds." *Physica C: Superconductivity* 221, no. 1-2 1995: 1-10. .

Lee, Peter, Mark Beno, Deming Shu, M Ramanathan, Joseph Mitchell, James Jorgensen and Robert Von Dreele. "Proposed dedicated high-resolution powder diffraction beamline at the Advanced Photon Source." Paper presented at the 8th International Conference on Synchrotron Radiation Instrumentation (SRI 2003), San Francisco, CA, August 25, 2003 - August 29, 2003.

Lee, Peter, Mark Beno, Robert Von Dreele, Deming Shu, Charles Kurtz, Guy Jennings, James Jorgensen and et al. "11-BM, a dedicated high-resolution powder diffraction beamline at Advanced Photon Source." Paper presented at the 2004 Denver X-ray Conference, Steamboat Springs, CO, August 2, 2004 - August 6, 2004.

Lee, Peter, Y Zhang and Robert Von Dreele. "Powder diffraction at Advanced Photon Source : now and future." Paper presented at the Annual National Meeting of the American Crystallographic Association, Chicago, IL, July 17, 2004 - July 22, 2004.

---



Madden, Timothy, Robert Von Dreele, Brian Toby, Jonathan Baldwin and Matthew Suchomel. "Scanning CCD for X-ray Powder Diffraction." Paper presented at the SRI 2013, Gaithersburg, MD, June 19, 2013 - June 21, 2013.

Madden, Timothy, Robert Von Dreele, Brian Toby, Matthew Suchomel, Jonathan Baldwin and John Weizeorick. "Scanning high resolution CCD detector for powder diffraction." Paper presented at the APS User Meeting, Argonne, IL, May 7, 2012 - May 10, 2012.

Margiolaki, I, J Wright, A Fitch, G Fox, A Labrador, Robert Von Dreele, K Miura, "Powder diffraction studies on proteins : An overview of data collection approaches." Paper presented at the European Powder Diffraction Conference (EPDIC-10), Geneva, Switzerland, September 1, 2006 - September 4, 2006.

Shu, Deming, Peter Lee, Curt Preissner, M Ramanathan, Mark Beno, Robert Von Dreele, R Raney, "Mechanical design of a high-resolution x-ray powder diffractometer at the Advanced Photon Source." Paper presented at the SPIE Optics and Photonics 2007, San Diego, CA, August 26, 2007 - August 30, 2007.

Shu, Deming, Peter Lee, M Ramanathan, Mark Beno, Robert Von Dreele, R Raney, Lynn Ribaud, "Mechanical design of a high-resolution x-ray powder diffractometer at the Advanced Photon Source." Paper presented at the SPIE Optics and Photonics 2007, San Diego, CA, August 26, 2007 - August 30, 2007.

Toby, Brian, Timothy Madden, Matthew Suchomel, Jonathan Baldwin, Robert Von Dreele. "A Scanning CCD Detector for Powder Diffraction Measurements." *Journal of Applied Crystallography* (forthcoming).

Toby, Brian, Robert Von Dreele. "GSAS-II: the genesis of a modern open-source all-purpose crystallography software package." *Journal of Applied Crystallography* (forthcoming).

Toby, Brian, Robert Von Dreele. "What's New in GSAS-II." *Powder Diffraction* 29, no. S2 Dec, 2014: S2-S6. doi: 10.1017/S0885715614000736.

Vogel, S, C Hartig, L Lutterotti, Robert Von Dreele, H Wenk, D Williams. "Texture measurements using the new neutron diffractometer HIPPO and their analysis using the Rietveld method." *Powder Diffraction* 10, no. 1 Mar, 2004: 65-8. .

Von Dreele, Robert. "Powder Diffraction: What's in a Name?." *Acta Crystallographica. Section C: Crystal Structure Communications* (forthcoming).

Von Dreele, Robert. "Binding of N-acetylglucosamine oligosaccharides to hen egg white lysozyme : a powder diffraction study." *Acta Crystallographica. Section D* D61 2005: 22-32. doi: 10.1107/S0907444904025715.

Von Dreele, Robert. "Protein crystal structure determination from powder diffraction data." Paper presented at the NSLS Users Meeting Workshop "Bio-Matters: From Infrared to X-Rays", Upton, NY, May 21, 2003.

Von Dreele, Robert. "Characterization of proteins by powder diffraction." Paper presented at the 11th European Powder Diffraction Conference (EPDIC-11), Warsaw, Poland, September 19, 2008 - September 22, 2008.

Von Dreele, Robert. "A rapidly filled capillary mount for both dry powder and polycrystalline slurry samples." *Journal of Applied Crystallography* 39, no. Pt. 1 Feb, 2006: 124-126. .

Von Dreele, Robert. "Multipattern Rietveld refinement of protein powder data : an approach to higher resolution." *Journal of Applied Crystallography* 40 2007: 133-143. doi: 10.1107/S0021889806045493.

Von Dreele, Robert. "Rietveld refinement for parametric powder diffraction : SeqGSAS and Seqplot." *Commission on Powder Diffraction Newsletter* (forthcoming).

Von Dreele, Robert. "Small Angle Scattering Data Analysis in GSAS-II." *Journal of Applied Crystallography* 47 2014: 1784-1789. doi: 10.1107/S1600576714018366.

Von Dreele, Robert. "5.2 Data Processing - powder diffraction peak profiles." (forthcoming).

Von Dreele, Robert. "Accuracy in Powder Diffraction - 'Are We There Yet?'" *LEGACY DEFAULT JOURNAL* (forthcoming).

Von Dreele, Robert, Pei-Lun Lee. "Protein powder diffraction in a hurry." Paper presented at the NSLS Users Mtg. Workshop "Frontiers in Powder Diffraction", Upton, NY, May 19, 2003.

Von Dreele, Robert, Peter Lee, Y Zhang. "Protein polycrystallography." Paper presented at the European Powder Diffraction Conference, Prague, Czech Republic, November 2, 2004 - November 5, 2004.

Von Dreele, Robert, Brian Toby. "X-ray powder diffraction." (forthcoming).

Von Dreele, Robert, T Uchida, Y Wang, N Nishiyama, K Funakoshi, A Nozawa, Mark Rivers, "Non-cubic crystal symmetry of CaSiO<sub>3</sub> perovskite up to 18 GPa and 1600K." *Earth and Planetary Science Letters* 282 2009: 268-274. doi: 10.1016/j.epsl.2009.03.027.

Wang, J, Brian Toby, Peter Lee, Lynn Ribaud, Sytle Antao, Charles Kurtz, M Ramanathan, et al."A dedicated powder diffracton beamline at the Advanced Photon Source : Commissioning and early operational results." *Review of Scientific Instruments* 79 2008: 08515. doi: 10.1063/1.2969260.

Wang, Y, T Uchida, N Nishiyama, Robert Von Dreele, M Rivers, K Funakoshi, A Nozawa, et al."A new technique for angle-dispersive powder diffraction using an energy-dispersive setup and synchrotron radiation." *Journal of Applied Crystallography* 37, no. Pt. 6 Dec, 2004: 947-56. .

Wang, Y, T Uchida, Robert Von Dreele, M Rivers, N Nishyama, A Nozawa, H Kaneko, et al."CAESAR: A technique for angle-dispersive powder diffraction using an energy-dispersive setup and white synchrotron radiaiton." Paper presented at the , null, null.

Zhang, Y, J Harper, Peter Lee, Robert Von Dreele, D Grant. "Ab initio structure determination of ambic acid with synchrotron powder diffraction and solid-state NMR."Argonne National Laboratory, ANL-03/21, December 2003 .

Zlotoyabko, E, Elad Caspi, Joseph Fieramosca, Robert Von Dreele, F Marin, G Mor, Y Politi, et al."The differnces between bond lengths in biogenic and geologocal calcite." *Crystal Growth & Design* 10, no. 3 2010: 1207-1214. doi: 10.1021/cg901195t.