

## Katharine Page

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### Research

An understanding of many materials phenomena of interest today calls for *observation* of atomic-level structure, based on sophisticated scattering techniques. My research focuses on new insights into complex functional materials, both bulk and nano, through advances in structural characterization.

### Education

**2004–2008** PhD in Materials, University of California Santa Barbara (with Ram Seshadri and Anthony K. Cheetham FRS). PhD thesis titled, *Local Structure Investigation of Bulk and Nanophase Perovskites*.

**2000–2004** B.S. in Chemical Engineering, University of Maine.

### Employment

**2014– present** Diffraction Instrument Scientist, Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN.

**2011– 2014** NPDF Instrument Scientist and Total Scattering Team Leader, Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, NM.

**2009–2011** Director's Postdoctoral Fellow with Dr. Thomas Proffen, Los Alamos National Laboratory, Los Alamos, NM.

**Summer 2005** Materials Scientist Internship with Dr. Mark Hampden-Smith, Cabot Superior Micropowders, Albuquerque, NM.

**Summers 2002, 2003, 2004** Pre-Doctoral Researcher with NASA Undergraduate Student Research, NASA Glenn Research Center (2002) and Los Alamos National Laboratory (2003–2004).

**Summer 2001** Pre-Doctoral Researcher, with Dr. William DeSisto at the Surface Science and Technology Laboratory University of Maine, Department of Chemical Engineering.

### Awards and Honors

**2018** Neutron Scattering Society of America Distinguished Service Award.

**2015** Department of Energy Office of Science Early Career Research Program Award Winner.

**2010** Los Alamos National Laboratory Postdoctoral Research Day Outstanding Poster Award Winner.

**2008** Los Alamos National Laboratory Director's Postdoctoral Fellowship.

**2008** Neutron Scattering Society of America Prize for Outstanding Student Research.

**2006** National Science Foundation Graduate Research Fellowship.

2006 American Crystallographic Association Margaret C. Etter Student Lecturer Award.

2006 NASA Harriet G. Jenkins Graduate Student Fellowship Recipient.

2005 National Science Foundation Integrative Graduate Education and Research Traineeship Fellowship.

## Publications

[Google Scholar Link](#)

### Submitted or in Press

106. D. Wendt, E. Bozin, J. Neufeind, K. Page, W. Ku, L. Wang, B. Fultz, A. Tkachenko, I. Zaliznyak, Entropic elasticity and negative thermal expansion in a simple cubic crystal, submitted.
105. J. Zhang, J. Yan, S. Calder, Q. Zheng, M. Qiang, M. McGuire, D. Abernathy, Y. Ren, S. Lapidus, K. Page, H. Zheng, J. Freeland, J. Budai, and R. Hermann, Antiferromagnetism in a rocksalt high entropy oxide, submitted.
104. D. Hobbis, R. P. Hermann, H. Wang, D. S. Parker, T. Pandely, J. Martin, K. Page, and G. S. Nolas, Structural, chemical, electrical, and thermal properties of n-type NbFeSb, submitted.
103. B. Sun, S. Niu, N. Shulumba, K. Page, K. Mahalingam, J. Milam-Guerrero, B. Zhao, R. Haiges, M. Mecklenburg, B. C. Melot, Y.-D. Jho, B. M. Howe, M. E. Manley, J. Ravichandran, A. J. Minnich, Ultralow glass-like thermal conductivity in hexagonal perovskite chalcogenide single crystals, submitted.
102. E. Zhao, M. Zhang, X. Wang, E. Hu, J. Liu, X. Yu, Y. Xia, M. Olguin, T. A. Wynn, Y. S. Meng, K. Page, F. Wang, H. Li, X.-Qing Yang, L. Chen, and X. Huang, Origin of the stable and reversible lattice oxygen redox in Li-rich layered oxides, submitted.
101. X. Yu, E. Hu, X. Wang, F. Meng, J. Liu, J.-N. Zhang, K. Page, W. Xu, L. Gu, R. Xiao, H. Li, X. Huang, L. Chen, X.-Q. Yang, Nature of shortened O-O pair without bonding and its relationship with oxygen redox contribution in highly charged LiCoO<sub>2</sub>, submitted.
100. H. Zhang, S. Liu, C. Nelson, L. N. Bezmaternykh, Y.-S. Chen, SY. Wang, R. Lobo, K. Page, M. Matsuda, D. Pajerowski, and T. J. Williams, Structural features enabling multiferroic behavior in the RX<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> system, submitted.
99. S. M. Clark, B. Colas, D. Jacob, J. Neufeind, H.-W. Wang, K. Page, and A. K. Soper, Nano-crystalline fluid controls carbonate bio-mineralization, submitted.
98. Y. Shi, J. Neufeind, D. Ma, K. Page, L. A. Lamberson, N. J. Smith, A. Tandia, A. P. Song, Ring size distribution of silicate glasses determined by neutron scattering first sharp diffraction peak analysis, submitted.
97. K. Kupwade-Patil, P. J. Boul, D. K. Rasner, S. M. Everett, T. Proffen, K. Page, D. Ma, D. Olds, C. J. Thaemlitz, and O. Bykztrk, Retarder effect on hydrating oil well cements investigated using in situ neutron/x-ray pair distribution function analysis, submitted.
96. D. Samrouni, H.-W. Wang, S. B. Clark, C. Pearce, K. Page, D. J. Wesolowski, A. G. Stack, and A. E. Clark, Molecular speciation based decomposition of neutron and x-ray scattering - a case study of concentrated NaOH, *Phys. Chem. Chem. Phys.*, **accepted** (2019).
95. B. Song, E. Hu, J. Liu, Y. Zhang, X.-Qing Yang, N. Jagjit, A. Huq, and K. Page, P3-type Na<sub>2/3</sub>Mg<sub>1/3</sub>Mn<sub>2/3</sub>O<sub>2</sub> as a high capacity and low-cost sodium-ion cathode using oxygen redox reaction, *J. Mater. Chem. A*, **in press** (2019). [DOI Link](#)

94. F. Polo-Garzon, S. Luo, Y. Cheng, L. L. Daemen, K. Page, A. J. Ramirez-Cuesta, P. F. Britt, and Z. Wu, Neutron scattering investigations of hydride species in heterogeneous catalysis, *ChemSusChem*, **in press** (2018). [DOI Link](#)

### Published

93. A. Bernasconi, K. Page, Z. Dai, L. Tan, A. Rappe, and L. Malavasi, Ubiquitous short-range distortion of hybrid perovskites and hydrogen bonding role: the MAPbCl<sub>3</sub> case, *J. Phys. Chem. C*, **122** (2018) 28265–28272. [DOI Link](#)
92. T. Graham, D. Semrouni, E. A. Ramirez-Cuesta, K. Page, A. Clark, G. Schenter, C. Pearce, A. Stack, and H.-W. Wang, Coupled multimodal dynamics of hydrogen-containing ion networks in water-deficient, sodium-hydroxide-aluminate solutions, *J. Phys. Chem. B*, **122** (2018) 12097–12106. [DOI Link](#)
91. X. Zhang, P. Huestis, C. I. Pearce, J. Hu, K. Page, L. M. Anovitz, A. B. Aleksandrov, M. P. Prange, S. Kerisit, M. E. Bowden, W. Cui, Z. Wang, N. R. Jaegers, T. R. Graham, M. Dembowski, H.-Wen Wang, J. Liu, A. T. N'Diaye, M. Bleuel, D. Mildner, T. M. Orlando, G. A. Kimmel, J. A. La Verne, S. B. Clark, and K. M. Rosso, Boehmite and gibbsite nanoplates for synthesis of advanced alumina product, *ACS Appl. Nano Mater.*, **1** (2018) 7115–7128. [DOI Link](#)
90. Z. Wu, S. Lan, X. Wei, K. Page, D. Olds, B. Shen, and X.-L. Wang, Heterogeneous nucleation in Zr-Cu-Al-Ag metallic glasses triggered by quenched-in metastable crystals - a time-resolved neutron diffraction study, *Physica B*, **551** (2018) 60–63. [DOI Link](#)
89. K. Page, B. Haberl, L. Coates, M. Tucker, Preface: Special topic on advances in modern neutron diffraction at Oak Ridge National Laboratory, *Rev. Sci. Instrum.*, **89** (2018) 092601. [DOI Link](#)
88. D. Olds, R. A. Mills, M. T. McDonnell, J. Liu, J. R. Kim, M. T. Dunstan, M. W. Gaultois, S. M. Everett, M. G. Tucker, and K. Page, A high temperature gas flow environment for neutron total scattering studies of complex materials, *Rev. Sci. Instrum.*, **89** (2018) 092906. [DOI Link](#)
87. T.-M. Usher, J. S. Forrester, M. McDonnell, J. Neuefeind, K. Page, P. Peterson, I. Levin, and J. L. Jones, Time of flight neutron total scattering with applied electric field: *ex situ* studies of ferroelectric materials, *Rev. Sci. Instrum.*, **89** (2018) 092905. [DOI Link](#)
86. C. E. White, N. Garg, D. Olds, J. Vocaturo, M. Everett, and K. Page, A uniaxial load frame for *in situ* neutron studies of stress-induced changes in cementitious materials and related systems, *Rev. Sci. Instrum.*, **89** (2018) 092903. [DOI Link](#)
85. S. Calder, K. An, R. Boehler, C. R. Dela Cruz, M. D. Frontzek, M. Guthrie, B. Haberl, A. Huq, S. A. J. Kimber, J. Liu, J. Molaison, J. Neuefeind, K. Page, A. M. dos Santos, K. M. Taddei, C. Tulk and M. G. Tucker, A suite-level review of the neutron powder diffraction instruments at Oak Ridge National Laboratory, *Rev. Sci. Instrum.*, **89** (2018) 092701. [DOI Link](#)
84. A. M. dos Santos, J. Molaison, B. Haberl, L. Krishna, K. Page, M. Loguillo and X. Wang, The high pressure gas capabilities at Oak Ridge National Laboratory's neutron facilities, *Rev. Sci. Instrum.*, **89** (2018) 092907. [DOI Link](#)
83. L. Yu, R. Han, X. Sang, J. Liu, B. M. Hudak, A. Patel, K. Page, and B. S. Guiton, Independent control of structure, composition, and morphology in the creation of hollow iron oxide nanocapsules, *ACS Nano*, **12** (2018) 9051–9059. [DOI Link](#)
82. P. Zhanga, J. Liu, K. Page, and A. Navrotsky, Calorimetric study of the thermodynamic properties of Mn<sub>5</sub>O<sub>8</sub>, *J. Am. Ceram. Soc.* (2018) 00:1–8. [DOI Link](#)
81. X. Zhang, W. Cui, K. Page, C. I. Pearce, M. E. Bowden, T. R. Graham, Z. Shen, P. Li, Z. Wang, S. Kerisit, A. T. N'Diaye, S. B. Clark, and K. M. Rosso, Size and morphology controlled synthesis of boehmite nanoplates and crystal growth mechanisms, *Cryst. Growth Des.*, **18** (2018) 3596–3606. [DOI Link](#)

80. H.-W. Wang, L. Vlcek, J. C. Neufeind, K. Page, S. Irle, J. M. Simonson, and A. G. Stack, Decoding oxyanion aqueous solvation structure: a potassium nitrate example at saturation, *J. Phys. Chem. B*, **122** (2018) 7584-7589. [DOI Link](#)
79. S. Sarker, D. Isheim, G. King, Q. An, D. Chandra, S. I. Morozov, K. Page, J. N. Wermer, D. N. Seidman M. Dolan, Icosahedra clustering and short range order in Ni-Nb-Zr amorphous membranes, *Sci. Rep.*, **8** (2018) 6084. [DOI Link](#)
78. T.-M. Usher, D. Olds, J. Liu, and K. Page, A numerical method for deriving shape function of nanoparticles for pair distribution function refinements, *Acta Cryst. A*, **74** (2018) 322–331. [DOI Link](#).
77. D. Olds, C. N. Saunders, M. Peters, T. Proffen, J. Neufeind, and K. Page, Precise implications on real-space PDF modeling from effects intrinsic to modern time of flight neutron diffractometers, *Acta Cryst. A*, **74** (2018) 322–331. [DOI Link](#).
76. J. Liu, L. Yu, E. Hu, B. S. Guiton, X.-Q. Yang, and K. Page, Large scale synthesis and comprehensive structure study of  $\delta$ -MnO<sub>2</sub>, *Inorg. Chem.*, **57** (2018) 6873–6882. [DOI Link](#)
75. X. Rong, J. Liu, E. Hu, Y. Liu, Y. Wang, J. Wu, X. Yu, K. Page, Y.-S. Hu, W. Yang, H. Li, X.-Q. Yang, L. Chen, and X. Huang, Structure-Induced Reversible Anionic Redox Activity in Na Layered Oxide Cathode, *Joule*, **2** (2018) 125–140. [DOI Link](#)
74. D. Olds, K. V. Lawler, A. A. Paecklar, J. Liu, K. Page, P. F. Peterson, P. M. Forster, and J. R. Neilson, Capturing the details of N<sub>2</sub> adsorption in zeolite X using stroboscopic isotope contrasted neutron total scattering, *Chem. Mater.*, **30** (2018) 296–302. [DOI Link](#)
73. D. Olds, P. F. Peterson, M. Crawford, J. R. Neilson, H.-W. Wang, P. S. Whitfield, and K. Page, Combinatorial appraisal of transition states for in situ pair distribution function analysis, *J. Appl. Cryst.*, **50** (2017) 1744–1753. [DOI Link](#)
72. D. H. Fabini, T. A. Siaw, C. C. Stoumpos, G. Laurita, D. Olds, K. Page, J. G. Hu, M. G. Kanatzidis, S. Han, R. Seshadri, Universal Dynamics of Molecular Reorientation in Hybrid Lead Iodide Perovskites, *J. Am. Chem. Soc.*, **139** (2017) 16875–16884. [DOI Link](#)
71. E. S. Muckley, M. Naguib, H.-W. Wang, L. Vlcek, N. C. Osti, R. L. Sacci, X. Sang, R. R. Unocic, Y. Xie, M. Tyagi, E. Mamontov, K. Page, P. R. C. Kent, J. Nanda, and I. N. Ivanov, Multimodality of structural, electrical, and gravimetric responses of intercalated MXenes to water, *ACS Nano*, **11** (2017) 11118–11126. [DOI Link](#)
70. J. Shamblin, Z. Dun, M. Lee, S. Johnston, E. S. Choi, K. Page, Y. Qiu, H. Zhou, Structural and magnetic short-range order in fluorite Yb<sub>2</sub>TiO<sub>5</sub>, *Phys. Rev. B*, **96** (2017) 174418. [DOI Link](#)
69. H. Nakotte, C. Silkwood, K. Page, H. W. Wang, D. Olds, B. Kiefer, S. Manna, D. Karpov, E. Fohntung, and E. E. Fullerton, Pair distribution function analysis applied to decahedral gold nanoparticles, *Phys. Scripta*, **92**, 114002. [DOI Link](#)
68. S. Zhou, E. S. Howard, J. Liu, N. H. Bashian, K. Nolan, S. Krishnamoorthy, G. M. Rangel, M.-T. Sougrati, G. K. S. Prakash, K. Page, and B.C. Melot, Hydrothermal preparation, crystal chemistry, and redox properties of iron muscovite clay, *ACS Appl. Mater. Interfaces*, **9** (2017) 34024-34032. [DOI Link](#)
67. R. Wang, A. Gebretsadik, S. Ubaid-Kassis, A. Schroeder, T. Vojta, P. J. Baker, F. L. Pratt, S. J. Blundell, T. Lancaster, I. Franke, J. S. Moller, and K. Page, Quantum Griffiths phase inside the ferromagnetic phase of Ni<sub>1-x</sub>V<sub>x</sub>, *Phys. Rev. Lett.*, **118** (2017) 267202. [DOI Link](#)
66. J. Liu, D. Olds, R. Peng, L. Yu, G. S. Foo, S. Qian, J. Keum, B. S. Guiton, Z. Wu, and K. Page, Quantitative analysis of the morphology of 101 and 001 faceted anatase TiO<sub>2</sub> nanocrystals and its implication on photocatalytic activity, *Chem. Mater.*, **29** (2017) 5591-5604. [DOI Link](#)

65. L. K. Lamontagne, G. Laurita, M. Knight, H. Yusuf, J. Hu, R. Seshadri, and K. Page, The role of structural and compositional heterogeneities in the insulator-to-metal transition in hole-doped  $\text{APd}_3\text{O}_4$  (A= Ca, Sr), *Inorg. Chem.*, **56** (2017) 5158-5164. [DOI Link](#)
64. D. Olds, K. Page, A. Paecklar, P. F. Peterson, J. Liu, G. Rucker, M. Ruiz-Rodriguez, M. Olsen, M. Pawel, S. H. Overbury, and J. R. Neilson, A high precision gas flow cell for performing in situ neutron studies of local atomic structure in catalytic materials, *Rev. Sci. Instrum.*, **88** (2017) 034101. [DOI Link](#)
63. C. E. White, D. P. Olds, M. Hartl, R. P. Hjelm, K. Page, Evolution of the pore structure during the early stages of the alkali-activation reaction: an in situ small-angle neutron scattering investigation, *J. Appl. Cryst.*, **50** (2017) 61-75. [DOI Link](#)
62. D. S. Charles, M. Feygenson, K. Page, J. Neuefeind, W. Xu, and X. Teng, Structural water engaged disordered vanadium oxide nanosheets for high capacity aqueous potassium-ion storage, *Nat. Commun.*, **8**, (2017) 15520. [DOI Link](#)
61. H.-W. Wang, L. Daemen, M. C. Cheshire, M. K. Kidder, A. G. Stack, L. F. Allard, J. Neuefeind, D. Olds, J. Liu, and K. Page, Synthesis and structure of synthetically pure and deuterated amorphous (basic) calcium carbonates, *Chem. Commun.* **53** (2017) 2942-2945. [DOI Link](#)
60. Y. Xu, M. Feygenson, K. Page, L. S. Nickles, K. S. Brinkman, Structural evolution in hollandite solid solutions across the A-site compositional range from  $\text{Ba}_{1.33}\text{Ga}_{2.66}\text{Ti}_{5.34}\text{O}_{16}$  to  $\text{Cs}_{1.33}\text{Ga}_{1.33}\text{Ti}_{6.67}\text{O}_{16}$ , *J. Am. Ceram. Soc.*, **99**, (2017) 4100-4106. [DOI Link](#)
59. K. Page, J. E. Siewenie, P. Quadrelli, and L. Malavasi, Short-range order of methylammonium and persistence of distortion at the local scale in  $\text{MAPbBr}_3$  hybrid perovskite, *Angew. Chem.*, **128** (2017) 14532-14536. [DOI Link](#)
58. P. Whitfield, N. Herron, W. E. Guise, K. Page, Y.Q. Cheng, I. Milas, and M. K. Crawford, Structures, phase transitions, and tricritical behavior of the hybrid perovskite methyl ammonium lead iodide, *Sci. Rep.*, **6** (2017) 35685. [DOI Link](#)
57. J. Liu, A. Huq, Z. Moorhead-Rosenberg, A. Manthiram, and K. Page, Nanoscale Ni/Mn ordering in the high voltage spinel cathode  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ , *Chem. Mater.*, **28** (2016) 6817–6821. [DOI Link](#)
56. P. Metz, R. Koch, B. Cladek, K. Page, J. Neuefeind, and S. Misture, X-ray and neutron total scattering analysis of  $\text{H}_y \cdot (\text{Bi}_{0.2}\text{Ca}_{0.55}\text{Sr}_{0.25})(\text{Ag}_{0.25}\text{Na}_{0.75})\text{Nb}_3\text{O}_{10} \cdot x\text{H}_2\text{O}$  perovskite nanosheet booklets with stacking disorder, *Powder Diffr.*, **31** (2016) 126-134. [DOI Link](#)
55. J. E. Douglas, E. E. Levin, T. M. Pollock, J. C. Castillo, P. Adler, C. Felser, S. Krmer, K. L. Page, and R. Seshadri, Magnetic hardening and antiferromagnetic/ferromagnetic phase coexistence in  $\text{Mn}_{1-x}\text{Fe}_x\text{Ru}_2\text{Sn}$  Heusler solid solutions, *Phys. Rev. B*, **94**, 094412. [DOI Link](#)
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52. M. Hartl, S. Carlson, Y. Lee, G. Muhrer, R. C. Gillis, T. Huegle, E. Iverson, L. Daemen, Y. Cheng, T. Ramirez-Cuesta, D. Olds, and K. Page, Hydrogen adsorption on catalyst surfaces for the ortho- to parahydrogen conversion, *Phys. Chem. Chem. Phys.*, **18** (2016) 17281-17293. [DOI Link](#)
51. H.-W. Wang, M. Naguib, K. Page, D. J. Wesolowski, Y. Gogotsi, Resolving the Structure of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXenes through multilevel structural modeling of the atomic pair distribution function, *Chem. Mater.*, **28** (2016) 349–359. [DOI Link](#)

50. G. Laurita, K. Page, S. Suzuki, and R. Seshadri, Average and local structure of the Pb-free ferroelectric perovskites (Sr,Sn)TiO<sub>3</sub> and (Ba,Ca,Sn)TiO<sub>3</sub>, *Phys. Rev. B*, **92** (2015) 214109. [DOI Link](#)
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37. C. E. White, N. J. Henson, L. L. Daemen, M. Hartl, and K. Page, Uncovering the True Atomic Structure of Disordered Materials: The Structure of a Hydrated Amorphous Magnesium Carbonate, *Chem. Mater.*, **26** (2014) 2693– 2702. [DOI Link](#)
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23. K. Page, C. E. White, Eben G. Estell,\* A. Llobet, Th. Proffen, Treatment of hydrogen background in bulk and nanocrystalline neutron total scattering experiments, *J. Appl. Cryst.*, **44** (2011), 532–539. [DOI Link](#)
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21. K. Page, T. C. Hood, T. Proffen, and R. B. Neder, Building and refining complete nanoparticle structures with total scattering data, *J. Appl. Cryst.* **44** (2011), 327–336. [DOI Link](#)

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16. K. Page, T. Kolodiaznyi, Th. Proffen, A. K. Cheetham, and R. Seshadri, Distinct local structures of Nb-substituted SrTiO<sub>3</sub> and BaTiO<sub>3</sub> from total neutron scattering: Implications for electronic properties, *Phys. Rev. Lett.* **101** (2008) 205502(1–4). [DOI Link](#)
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8. Y. -I. Kim, K. Page, and R. Seshadri, Synchrotron X-ray study of polycrystalline wurtzite Zn<sub>1-x</sub>Mg<sub>x</sub>O (0 ≤ x ≤ 0.15): Evolution of crystal structure and polarization, *Appl. Phys. Lett.* **90** (2007) 101914 (1-3). [DOI Link](#)
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6. G. Lawes, B. Melot, K. Page, C. Ederer, M. A. Hayward, Th. Proffen, and R. Seshadri, Dielectric anomalies and spiral magnetic order in CoCr<sub>2</sub>O<sub>4</sub>, *Phys. Rev. B* **74** (2006) 024413(1-6). [DOI Link](#)
5. Th. Proffen, K. L. Page, S. E. McLain, B. Clausen, T. W. Darling, J. A. TenCate, E. Ustundag, and S. Y. Lee, Atomic pair distribution function analysis of materials containing crystalline and amorphous phases, *Z. Kristallogr.* **220** (2005) 1002-1008. [DOI Link](#)



4. K. Page, Th. Proffen, H. Terrones, M. Terrones, L. Lee, Y. Yang, S. Stemmer, R. Seshadri, and A. K. Cheetham, Direct observation of the structure of gold nanoparticles by total scattering powder neutron diffraction, *Chem. Phys. Lett.* **393** (2004) 385-388. [DOI Link](#)
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2. Th. Proffen and K. L. Page, Obtaining structural information from the atomic pair distribution function, *Z. Kristallogr.* **219** (2004) 130-135. [DOI Link](#)
1. J. C. Hermanson, H. Johari, D. P. Stocker, U. G. Hegde, E. Ghaem-Maghani, and K. L. Page, Thermal characteristics and structure of fully-modulated, turbulent diffusion flames in microgravity, *AIAA* (2004) 0959(1-10).

## Book Chapters

- K. Page, Th. Proffen, and R. B. Neder. *Structure of Nanoparticles from Total Scattering*. In E.J. Mittermeijer, editor, *Modern Diffraction Methods*, Weinheim, October 2012. Wiley Verlag GmbH.
- E. Moshopoulou, P. Foury-Leylekian, K. Page, C. Doubrovsky, M. Greenblatt, and A. Hurd, *Neutron and Synchrotron X-Ray Scattering Studies of Bulk and Nanostructured Multiferroic and Ferroelectric Materials*, In M. Alguer, J. M. Gregg, and L. Mitoseriu, editors, *Nanoscale Ferroelectrics and Multiferroics: Key Processing and Characterization Issues, and Nanoscale Effects*, May 2016. John Wiley Sons, Ltd.

## Invited Talks

- Invited Keynote Lecture, European Crystallographic Meeting, Vienna, Austria, August 2019.
- Probing catalytic interfaces with in situ neutron pair distribution function studies*, American Chemical Society Spring Meeting, Orlando, FL, April 2019.
- The influence of interlayer water on the structure and electrochemical performance of  $\delta$ -MnO<sub>2</sub>*, Materials Research Society Spring Meeting, Phoenix, AZ, April 2019.
- University of Illinois Urbana-Champaign Materials Department Colloquium, Urbana, IL, February 2019.
- Nanostructures and their interfaces: insights from neutron total scattering*, Center for Nanophase Materials Sciences Seminar Series, Oak Ridge, TN, November 2018.
- Probing solid-gas interfaces in situ with isotope contrasted neutron total scattering*, American Chemical Society Fall Meeting, Boston, MA, August 2018.
- Capturing nanoscale interfaces in action*, Gordon Research Conference on Solid State Chemistry, Gordon, NH, August 2018.
- DISCOVER: ORNLs Diffraction and Total Scattering Beamline for Materials Discovery*, 16th European Powder Diffraction Conference, Edinburgh, Scotland, July 2018.
- The influence of interlayer water on the structure and lithium intercalation ability of Cu-rich  $\delta$ -MnO<sub>2</sub>*, 2017 North American Solid State Chemistry Conference, Santa Barbara, CA, August 2017.
- Resolving the atomistic structure and morphology of functional nanomaterials*, International Union of Crystallography 2017, Hyderabad, India, August 2017.
- Capturing nanoscale structure and behavior in situ with neutron total scattering*, American Crystallographic Association Annual Meeting, Denver, CO, July 2016.
- Functional oxide materials in real and reciprocal space: resolving local and long-range atomic structures with TOPAS*, 13th TOPAS User Meeting, Bari, Italy, June 2016.

- Local structure and material interfaces: neutron PDF studies at the SNS*, SNS-HFIR User Meeting, Oak Ridge, TN, October 2015.
- Discovering the atomic structure of the world around us*, Santa Fe Alliance for Science Science Cafe, Santa Fe, NM, February 2014.
- Atomic structure studies for nanoscale material insights*, Materials Research Laboratory Outreach Program, Santa Barbara, CA, February 2014.
- Material insights from total scattering data: a tour of small box modeling*, Neutron and Nano User Meeting, Oak Ridge, TN, August 2013.
- Linking structure and function in finite materials*, 22nd International Materials Research Congress, Cancun, Mexico, August 2013.
- Total scattering developments for nanoscale materials characterization*, Advances in Powder Diffraction IV, Gaithersburg, MD, April 2013.
- Accelerating nanoscale research with neutron total scattering: linking structure and function in finite materials*, Annual Meeting of the Four Corners Section of the APS, Socorro, NM, October 2012.
- Probing nanostructure in functional materials with total scattering*, The 21st International Offshore (Ocean) and Polar Engineering Conference, Maui, HA, June 2011.
- Probing nanostructure in functional metal oxides with x-ray and neutron total scattering*, MS&T Conference, Houston, TX, October 2010.
- The continued impact of high resolution total scattering*, Denver X-ray Scattering Conference, Denver, CO, July 2010.
- Probing local structure in ferroelectric perovskites*, NSLS User Group Meeting, New York, May 2010.
- Probing nanoscale structural features in ferroelectric perovskites with the pair distribution function*, Electronic Materials and Applications 2010, Orlando, FL, January 2010.
- Local structure studies of oxynitrides, ferroelectric perovskite oxides and related materials* Pittsburgh Diffraction Conference, Athens, GA, October 2009.
- Pair Distribution Function Methods: Capabilities and Future Directions*, Information Science for Materials Design and Discovery, Los Alamos National Laboratory, NM, October 2009.
- Local structure in ferroelectric perovskites*, North American Solid State Chemistry Conference, Columbus, OH, June 2009.
- Local structure in ferroelectric perovskite oxides*, International Conference on Neutron Scattering, Knoxville, TN, May 2009.
- Probing size effects in functional metal oxide nanoparticles with the pair distribution function*, Materials Research Society Spring Meeting, San Francisco, CA, April 2009.
- Materials studies on the nanoscale with the pair distribution function technique*, American Conference on Neutron Scattering, Santa Fe, NM, May 2008.
- Total scattering and the local structure of polar inorganic materials*, Materials Department Winter Colloquium, Santa Barbara, CA, March 2008.
- Probing the local structure of functional bulk and nanomaterials*, Materials Research Laboratory Outreach Program, Santa Barbara, CA, February 2008.
- Pair distribution function analysis of nanosystems*, American Crystallographic Association Annual Meeting, Honolulu, HA, July 2006.

## Grants and Funding

- 2018** *Ammonia synthesis over 2D electride-based catalysts at ambient pressure and low temperature.* Oak Ridge National Laboratory, Laboratory Directed Research and Development Funding. Led by Zili Wu, Oak Ridge National Laboratory. US \$456,000. (Co-Investigator)
- 2018** *Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME).* The Department of Energy Office of Science, Office of Basic Energy Sciences Energy Frontier Research Center Program. US \$11,969,806. Led by Krista Walton, Georgia Institute of Technology. (Co-Investigator)
- 2018** *Advanced Neutron Characterizations for Biomass Catalysis.* The Department of Energy Office of Science, Bioenergy Technologies Office ChemCatBio Program. US \$100,000. (Principle Investigator)
- 2017** *Designing entropy-stabilized oxides and other chemically disordered materials: A stochastic, first principles-finite temperature approach.* Oak Ridge National Laboratory, Laboratory Directed Research and Development Funding. Led by Valentino Cooper, Oak Ridge National Laboratory. US \$470,259. (Co-Investigator)
- 2016** *Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)* The Department of Energy Office of Science, Office of Basic Energy Sciences Energy Frontier Research Center Program. US \$12,000,000. Led by Sue Clark, Pacific Northwest National Laboratory. (Co-Investigator)
- 2015** *Exploiting Small Signatures: Quantifying Nanoscale Structure and Behavior.* The Department of Energy Office of Science, Office of Basic Energy Science Early Career Research Program. US \$2,500,000. (Principle Investigator)
- 2015** *Chemical Reactivity of Solids: Chemical Dynamics of the Atomic Structure of Solids Using Time-of-Flight Neutron Total Scattering.* Oak Ridge National Laboratory, Laboratory Directed Research and Development Seed Funding. US \$190,000. (Principle Investigator)
- 2013-2015** *Probing Interface Reactions of Calcite Nanocrystals at Elevated Temperatures and Pressures.* Los Alamos National Laboratory, Laboratory Directed Research and Development Early Career Funding. US \$450,000. (Principle Investigator)
- 2013-2014** *Characterization of Phosphor Materials.* Work for Others Agreement with Toshiba Corporation, Tokyo, Japan. US \$250,000. (Principle Investigator)
- 2013** *Characterization of Glass Ceramic Materials.* Work for Others Agreement with Corning Incorporated, Corning, NY. US \$41,000. (Principle Investigator)
- 2012** *Development and Validation of In-Situ Probing Techniques to be Used at the Fission-Fusion Facility.* Los Alamos National Laboratory, Laboratory Directed Research and Development Reserve Funding. US \$251,000. (Co-Proposer with D. Brown)
- 2012** *7 Tesla Cryomagnet for Neutron Total Scattering,* LANL G&A Investment from Associate Directorate for Experimental Physical Sciences. US \$450,000. (Co-Proposer with A. Llobet)
- 2011-2012** *Hydrogen Storage Materials.* Work for Others Agreement with the National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan. US \$120,000. (Principle Investigator)

## Former Group Members (Current Location)

Postdoctoral Associate: Dr. Claire White (Civil and Environmental Engineering, Princeton University, Faculty)

Postdoctoral Associate: Dr. Hsiu-Wen Wang (Chemical Sciences Division, Oak Ridge National Laboratory, Research and Development Scientist)

Postdoctoral Associate: Dr. Daniel Olds (X-ray Scattering Division, Brookhaven National Laboratory, Beamline Scientist)

Postdoctoral Associate: Dr. Jue Liu (Neutron Scattering Division, Oak Ridge National Laboratory, Beamline Scientist)

Postdoctoral Associate: Dr. Tedi-Marie Usher-Ditzian (SCHOTT North America, Inc., Research and Development Scientist)

## Workshops, Outreach, and Service

Co-Organizer (with S. Rosencranz, B. Toby, B. Haberl, and M. Manley), *National School on Neutron and X-ray Scattering*, Oak Ridge, TN and Argonne, IL, June 2019.

Workshop Co-Organizer (with Thomas Proffen) and Lecturer, *Advanced structural characterization of nanomaterials*, American Crystallographic Association Annual Meeting, Cincinnati, OH, July 2019.

Tutorial Instructor, *Material insights from total scattering data: a tour of small box modeling and more*, Materials Research Society Spring Meeting Tutorial Session in Advances in *In Situ* Techniques for Diagnostics and Synthetic Design of Energy Materials, Phoenix, AZ, April 2019.

Co-Organizer (with S. Rosencranz, B. Toby, B. Haberl, B. Chakoumakos, J. Budai, and M. Manley), *National School on Neutron and X-ray Scattering*, Argonne, IL and Oak Ridge, TN, July/August 2018.

Organizing Committee and Co-Session Chair (with Kathleen Weigandt), *American Conference on Neutron Scattering*, College Park, MD, June 2018.

Committee Member, *NSLS-II High Energy Diffraction Proposal Review Panel*, Upton, NY, 2018-present.

Invited Instructor, *NSLS-II PDF Workshop*, Upton, NY, September 2018.

Co-Session Chair (with B. Frandsen), *Diffuse Scattering in Complex Oxides*, American Crystallographic Association Meeting, New Orleans, LA, August 2017.

Co-Session Chair (with E. Grenado), *Microsymposium on Total Scattering*, International Union of Crystallography, Hyderabad, India, August 2017.

Co-Organizer (with P. Khalifah) and Instructor, *Modern Methods in Rietveld Refinement for Structural Analysis*, Oak Ridge, TN, June 2017.

Co-Organizer (with M. Tucker, *et al.*) and Instructor, *US School on Total Scattering Analysis*, Oak Ridge, TN, May 2017 and August 2018.

Co-Organizer (with M. Tucker), *Discover Beam Line Workshop*, Oak Ridge, TN, May 2017.

Co-Session Chair (with J. Reibenspies), *Novel Measurements for Emerging Science*, American Crystallographic Association Meeting, Denver, CO, July 2016.

Instructor, *Modern Methods in Rietveld Refinement for Structural Analysis*, Tallahassee, FL, May 2015.

Co-Organizer (with M. Tucker and I. Levin), *RMCPProfile Workshop*, Oak Ridge, TN, February 2016.

Secretary, Neutron Scattering Society of America, 2015–present.

Consultant Member, International Union of Crystallography Commission on Powder Diffraction, 2014–present.

Local Co-Chair (with Z. Fisher), 2014 American Crystallographic Association Meeting, Albuquerque, NM, May 2014.

Invited Participant, Department of Energy *Quantum Condensed Matter Workshop*, Berkeley, CA, December 2013.

Neutron Special Interest Group Chair, American Crystallographic Association, 2013.

PhD Committee Member for J. Peterson, Physics Department, New Mexico State University, Las Cruces, NM, 2013.

Session Chair, *Nanomaterial Structure from Diffraction Data - II: Experimental Advances*, American Crystallographic Association Meeting, Honolulu, HI, July 2013.

Invited Participant, *Workshop for POWGEN Users*, Oak Ridge, TN, June 2013.

Co-Organizer (with C. E. White, Th. Proffen, M. Johnson, and N. J. Henson), *Advanced Simulation Techniques for Total Scattering Data Workshop*, Santa Fe, NM, October 2012.

Co-Session Chair (with Th. Proffen), *Local Structure and Partially Ordered Systems* and Workshop Instructor, *Modeling and Refinement of Nanoparticle Structures from Diffraction Data*, American Crystallographic Association Meeting, Boston, MA, July 2012.

Co-Host (with A. Llobet), *LANSCE User Group Meeting Workshop: New Directions in Total Scattering Research at LANSCE*, Los Alamos, NM, January 2012.

Committee Member, *ORNL Neutron Scattering Science Review*, Diffraction Category, Oak Ridge, TN, 2011–2014.

*Materials Structure and the Scale of Things*, Fifth grade outreach program to northern New Mexico schools with a grant from Los Alamos National Laboratory Community Outreach Programs, Los Alamos, NM, 2011-2013.

*Lujan Neutron Scattering School Lectures and Tutorial Sessions*, Lujan Neutron Scattering Center, Los Alamos, NM, January 2014, September 2012, July 2011, and August 2010.

*LANL Laboratory Directed Research and Development Proposal Review Committee Member*, Defects and Interfaces in Materials Category, Los Alamos, NM, April-July 2011.

*UC Santa Barbara Materials Research Laboratory External Advisory Board Member*, Santa Barbara, CA, December 2010 to present.

Session organizer and speaker at *UC Sponsored Lujan Workshop: Applications of Neutron Scattering to Materials and Earth Sciences*, Berkeley, CA, December 2010.

*Diffraction at Large Experimental Facilities*, University of California, Santa Barbara, CA, September 2010. (Lectures and tutorials with E. Rodriguez.)

*PDF Fitting: Practical Modeling Tutorial*, North American Solid State Chemistry Conference, Columbus, OH, June 2009. (Joint tutorial with Prof. V. Petkov, Central Michigan University.)

President, Los Alamos National Laboratory Postdoctoral Association, 2009-2010.

## Notable Extracurricular Accomplishments

**2003 - 2010** Nationally competitive Olympic style weightlifter. Earned numerous top five finishes at USA National and American Open Championships, 2008 Olympic Trials Participant. 2007, 2008 and 2009 Collegiate National Champion, 69 kg class.

**2000 - 2004** Division I varsity track athlete at the University of Maine. Received multiple top five finishes in the America East Conference indoor and outdoor track and field championships. Co-captain of varsity team for the 2002-2003 and 2003-2004 seasons, University discus record holder.

## Professional Memberships

American Crystallographic Association (ACA)  
American Chemical Society (ACS)  
Materials Research Society (MRS)  
Neutron Scattering Society of America (NSSA)

## References

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