

## *Curriculum Vitae*

### **Simon J. L. Billinge**

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#### **Professional Preparation**

University of Oxford,	Materials Science,	1986	BA
University of Pennsylvania	Materials Science and Eng.,	1992	Ph.D.
Los Alamos National Laboratory	Condensed Matter Physics,	1992 -1994	Postdoc

#### **Appointments**

2008-present	Professor of Materials Science and Applied Physics and Applied Mathematics, Columbia University
2008-present	Physicist, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory
2012	Long Term Visitor, Institute Laue Langevin, Grenoble, France
2011-2012	Long Term Visitor, European Synchrotron Radiation Facility, Grenoble, France
2003-2007	Professor of Physics, Michigan State University
2001-2002	Visiting Professor, University of Rome, 'La Sapienza'
1999-2003	Associate Professor of Physics, Michigan State University
1994-1999	Assistant Professor of Physics, Michigan State University
1992-1994	Director's Post-doctoral Research Fellow, Los Alamos National Laboratory

#### **Awards, and Honors**

2015	Texas A&M Clearfield Endowed Lecturer
2014	Fellow of the Neutron Scattering Society of America
2012	Neutron Scattering Society of America Service Award for outstanding service
2012	Editor of Acta Crystallographica Section A: Foundations of Crystallography
2011	Fulbright Research Scholar 2011-2012
2011	Carnegie Foundation of New York honored as one of 24 Outstanding Immigrants
2011	Co-editor of Journal Acta Crystallographica Section A: Foundations of Crystallography
2010	J. D. Hanawalt Award of the International Center for Diffraction Data
2007	University Distinguished Faculty Award, Michigan State University
2006	Fellow, American Physical Society
2006	Michigan State University, College of Nat. Sci., Distinguished Faculty Award
1998	Thomas H. Osgood Undergraduate Teaching Award
1995	Alfred P. Sloan Research Fellowship
1992	Sigma Xi Outstanding thesis award, U. Pennsylvania
1992	Electro-science Laboratories Award, U. Pennsylvania

#### **Societies**

American Physical Society, American Crystallographic Association, Materials Research Society, Neutron Scattering Society of America

#### **Current Research Interests**

Local structure property relationships of disordered crystals and nanocrystals using advanced x-ray and neutron diffraction techniques. Atomic Pair Distribution Function method applied to complex materials. Single crystal diffuse scattering and total scattering studies. Studies of charge localization and nanoscale inhomogeneous electronic states in complex electronic oxides. Studies of semiconductor alloys and microporous materials. Local structure of biologically relevant molecules and materials in the excited state. More information about my research, (p)reprints, and a complete publication list, can be found at <http://thebillingegroup.com/>

## **Professional and Synergetic Activities**

- Chairman** - *Chair, Materials Special Interest Group of the American Crystallographic Association 2015*  
*Chair, XPD beamline project Beamline Advisory Team (BAT) 2008-2014*  
*Chair Advanced Analysis of X-Ray and Neutron Scattering Data: Getting from data to science Workshop, Brookhaven National Laboratory, July 2013*  
*Chair, microsymposium on total pattern fitting, Accuracy in Powder Diffraction Conference, NIST 2013.*  
*Chair of the 2013 J.D. Hanawalt Prize selection committee of the ICDD*  
*Chair of the Joint US/Africa Materials Initiative Materials Research School, Addis Ababa, Ethiopia, 17<sup>th</sup> -22<sup>nd</sup> December 2012*  
*CoChair of ZING 2012 Nanoscience Conference, Lanzarote, February 2012*  
*Chair of the symposium "Amorphous, Activated and Nanomaterials" at the 10th Annual Pharmaceutical Powder X-ray Diffraction Symposium (PPXRD), Lyon, France, May 2011*  
*Chair of the microsymposium "SAXS/SANS, total scattering and the nanostructure problem" at the XXII congress of the International Union of Crystallography (IUCr), Madrid, Spain 2011*  
*CoChair, 2011 NSLS/CFN Joint Users' Meeting, Brookhaven National Laboratory, May 22-25<sup>th</sup> 2011*  
*Chair of the American Conference on Neutron Scattering, Ottawa, 2010*  
*Co-Chair of the NSF-DMR committee to Review the Center for High Resolution Neutron Scattering (CHRNS) at NIST, Gaithersburg, MD, October 2010*  
*Chair of the NSF-DMR committee to Review the Center for High Resolution Neutron Scattering (CHRNS) at NIST, Gaithersburg, MD, September 2009*  
*Chair of the International Conference on Neutron Scattering, Knoxville, NM, May 3 - 7<sup>th</sup> 2009*  
*Chair of the American Conference on Neutron Scattering, Santa Fe, NM, May 11-14<sup>th</sup> 2008*  
*NSF-DMR steering committee on Cyber-Infrastructure for the Materials Sciences (2005-2007)*  
*General Chair of the American Conference on Neutron Scattering, Chicago, IL, June 18-22<sup>nd</sup> 2006*  
*Workshop, Cyber Infrastructure for Materials Science, NSF supported workshop to identify CI needs for the materials science community, Washington DC, May 2006*  
*Continuing Education Committee of the American Crystallographic Association (2005-2007)*  
*Special Interest Group, American Crystallographic Association Neutron scattering (2001-2002) (elected position)*  
*Workshop, From Semiconductors to Proteins: beyond the average structure, Traverse City, MI, August 2001.*  
*Workshop, Local Structure from Diffraction, Traverse City, MI, July 1998.*
- Elected Positions** *Steering committee of the African Light Source (2015 - )*  
*Chair-elect, Materials Special Interest Group of the American Crystallographic Association 2014*  
*Co-editor of Journal Acta Crystallographica Section A: Foundations of Crystallography (2011-2020)*  
*Vice president, NSLS and NSLS-II user's executive committee (2010 – 2012)*  
*Vice President of the Neutron Scattering Society of America (2005-2010)*  
*Executive Committee of the International Commission on Powder Diffraction of the Union of Crystallography, (2005-2010)*  
*Executive Committee of the Advanced Photon Source Users Organization (2005-2007)*  
*Secretary of the Executive committee of the Neutron Scattering Society of America (2003-2005)*  
*Continuing Education Committee of the American Crystallographic Association (2003-2007)*

- Organizer - *Symposium "Electronic Oxides: Properties and Applications"*, CFMR spring symposium , Michigan State University, April 20th 1997.
- Co-organizer – *Symposium "Powder Pair Distribution Function and Pharmaceuticals"* at ACA annual meeting, Philadelphia, July 2015
- JUAMI symposium at the African-MRS*, Addis Ababa, Ethiopia, 10<sup>th</sup> December 2013
- Joint US/Africa Materials Initiative Materials Research School*, Addis Ababa, Ethiopia, 17<sup>th</sup> -22<sup>nd</sup> December 2012
- Symposium "Nanoscale Materials Diffraction"* at the NSLS/CFN users meeting, Brookhaven National Laboratory, Monday, May 24, 2010
- Workshop Beyond crystallography: Structure of nanostructured materials*, Tempe, AZ, May 17-21<sup>st</sup> 2008
- Workshop on PDF on the nanoscale*, ESRF, October 22-24<sup>th</sup> 2007.
- Symposium, "'Under the Bonnet' Powder Diffraction Software Workshop"*, European Powder Diffraction Conference, Geneva, Switzerland, September 1-4<sup>th</sup> 2006.
- Conference, "Structure of Nanocrystals"*, Tempe, AZ, December 5-8<sup>th</sup>, 2004.
- Workshop, "Local Atomic Structure Using Neutron Pair Distribution Function (PDF) Analysis"* at the American Conference on Neutron Scattering", College Park, MD, June 6-10th 2004.
- Symposium, "B. E. Warren Award Symposium"* at the 2003 annual meeting of the American Crystallographic Association, Cincinnati, July 2003.
- Workshop, "Real-space Pair Distribution Function Methods"* at the meeting "Neutrons In solid state Chemistry and the Earth Sciences Today and tomorrow (NICEST)", Oak Ridge, TN, March 2003.
- Symposia, "Impact of Scattering on Nanoscience and Nanotechnology"* and *"From Structures to Materials Science"*, at the annual meeting of the American Crystallographic Association, San Antonio, TX, May 2002.
- Workshop, "Real-space Pair Distribution Function Methods"*, at the annual meeting of the American Crystallographic Association 2001, Los Angeles, July 21-26 2001.
- Symposium, "Microstructure and Texture of Real Materials"*, at the XVIIIth International Union of Crystallography congress and General Assembly, Glasgow, Scotland, August 4th-13th 1999.
- Co-editor - Special Edition, *Nanoscale, Perovskites at the nanoscale: from fundamentals to applications* (with Josh Choi, 2015)
- Special edition, *MRS Bulletin on scattering* (with Paul Evans, July 2010 edition).
- Book, *Powder Diffraction: Theory and Practice*, (with Robert Dinnebier, RSC, 2008)
- Special edition, *Z. Kristallogr.* (with Thomas Proffen and Brian Toby 2003)
- Book, *From Semiconductors to Proteins: Beyond the Average Structure* (with Michael Thorpe, 2002).
- Book, *Local Structure From Diffraction* (with Michael Thorpe, 2002).
- Book, *Powder Diffraction: Theory and Practice* (with Robert Dinnebier, 2005).
- Co-Author - Book, 2<sup>nd</sup> Edition, *Underneath the Bragg-Peaks: structural analysis of complex materials* (with T. Egami, 2012).
- Book, *Underneath the Bragg-Peaks: structural analysis of complex materials* (with T. Egami, 2003).
- Review panels/committees –
- Advisory Committee, MICCoM (<http://miccom-center.org/>), computational materials science center Argonne National Laboratory (2016-)
- Triannual Review of Photon Sciences Division at SNS (2015)
- Review Panel for the ANL Director's Grand Challenge in "Big Data" (2013)
- User Working Group, XPDF beamline construction project, Diamond Light Source, UK (2013-2016)
- Advisory board member of the Materials Research Institute, Queen Mary's College, London (2013)
- NSF Focus group for Science and Engineering Gateways (2013)
- Program committee of the International Conference on Neutron Scattering, Edinburgh (2013)
- International Advisory Committee, International Conference on Communication, Computational

skills and Nanotechnology, Swami Ramanand Teerth Marathwada University, Nanded, Maharashtra State, India, January (2011)  
Visiting Committee, Energy Recovery Linac Project, Cornell University (2010,2012)  
Advisory Committee for the Expansion Initiative of the NIST Center for Neutron Research (NCNR), NIST (2010, 2011)  
DOE-BES review committee of Neutron Scattering Science Division at Oak Ridge National Laboratory (2010,2012)  
DOEANL Heavy Element Separation Site Review, Argonne, IL November 2009  
NSF-DMR review of the Center for High Resolution Neutron Scattering (CHRNS) at NIST, September 2009  
DOE-BES review committee of Neutron scattering at Oak Ridge National Laboratory (2009)  
NSF steering committee on Cyber-Infrastructure for the materials sciences (2005-2007)  
NSLS beamline review committee (with Eric Isaacs (chair), and J.D. Jorgensen), 2004  
NSF-MRI-IMR review panel, 2004  
NSF-CHRNS program review committee, 2004  
NSLS beamtime proposal review panel, 2002-2007  
ISIS facility access panel, 2005-2008

#### K-12 education and Outreach activities

Developed online peer-instruction platform for use in flipped classrooms, 2014  
Developed online research portal for JUAMI researchers (see below), 2013  
Organizer of an East African Materials Science Winter School, JUAMI, 2012  
Science Advisory Committee to the NSF funded PROMSE project to improve math and science education in the K-12 sector (2003-2010)  
Curriculum development for an AP course in nanotechnology at Everett High school in Lansing, MI, 2006-2007

## **Graduate Students**

**Current Students (date joined in brackets):** Chia-Hao Liu (July 2015), Soham Banerjee (June 2014), Maxwell Terban (Jan 2013).

#### **Graduated Ph.D.:**

**Columbia:** Chenyang Shi, (May 2012-August 2015), Xiaohao Yang (9/11-6/2015, JP Morgan Chase), Timur Dykhne (Columbia June 2011, Samsung, formerly Boston Consulting Group),  
**MSU:** Peng Tian (May 2010, Hutchin Hill Capital Hedge Fund) Ahmad Masadeh (January 2008, faculty position, U. Jordan), Hasan Yavas (October 2007, post-doc at Argonne National Lab), HyunJeong Kim (September 2007, post-doc at LANL. Now permanent position in Catalysis group in Japan) Moneeb Shatnawi (August 2007, faculty position, Hashemite U., Jordan), Mouath Shatnawi (May 2007, faculty position, U. Jordan), He Lin (Dec 2006, post-doc, Chinese synchrotron), Xiangyun Qiu (2004, post-doc Cornell U. Now faculty at George Washington U.), Emil Bozin, (May 2003, post-doc in the group. Now Assistant Scientist at Brookhaven National Laboratory), Peter Peterson (Dec. 2001, post-doc at Oak Ridge National Lab, now permanent at ORNL), Il-Kyoung Jeong (March 2001, post doc at Los Alamos National Lab, now faculty at Pohang U, Korea), Remo DiFrancesco (Dec. 1999, teaching faculty at Bloomburg College, PA)

**Masters Student research:** Neno Fuller (September 2015), Baruch Tabanpour (September 2014), Yarong Lin (spring 2014), Hrishi Tiwari (2010/11), Chenyang Shi (2010/11)

#### **Thesis committees (since 2014):**

*Thesis Defence:* Chris Gutierrez (2015, Physics), Zachariah Norman (2015, Chemistry), Yi Li (2015, MSE)  
*Thesis Proposal:* Max Terban (2015, MSE), Haixing Li (2015, MSE), Yi Li (2014, MSE)  
*Oral exam:* Jeff Taylor (2015, AP), Max Terban (2015, MSE)

## **Postdoctoral Fellows**

**Current:** Pavol Juhas (Assistant Scientist 12/11- ), Emil Bozin (Assistant Scientist, BNL, 2011-)

**Former:** Kirsten Jensen (10/13-09/15 Assistant Professor at U. Copenhagen, Denmark), Kevin Knox (07/11-04/15, JP Morgan Chase), Chung Koo Kim (04/2013-04/2015, Postdoc at BNL), Hefei Hu (03/13-09/14, Intel), Mirian Garcia-Fernandez (06/11-03/14, permanent staff, Diamond Light Source, UK), Milinda Abeykoon (10/09 – 13/05 permanent staff at BNL), Yingrui Shang (9/09-09/11 faculty position Tianjin University), Chris Farrow (09/07-06/11, permanent position at Enthought), Jiwu Liu (10/09-10/10, permanent position at Amazon.com), Emil Bozin (9/04-2/11, permanent position at Brookhaven National Laboratory), Wenduo Zhou (9/06-06/09, permanent position at ORNL), Asel Sartbaeva (2005-2007, Royal Society Research Fellow, Oxford University), Gianluca Paglia (6/04-6/06, permanent position in a company in Perth, Australia), Marek Schmidt (2/02-12/04, permanent position at Rigaku), Jacques Bloch (9/04-3/05, Post Doc, U. Regensburg), Mohamed Kemali (10/00-3/02, unknown), Matthias Gutmann (1/99 – 1/01, permanent position, ISIS, UK), Valeri Petkov (1999-8/02, faculty position, Central Michigan University), Thomas Proffen, (5/98-1/01, permanent position LANL. Now group leader at ORNL), Farida Mohiuddin-Jacobs (9/95-8/97, raising a family)

### **Visiting scientists**

Dr. Ann-Christin Dippel (August 2014, DESY, Hamburg), Dr. Partha Das (July 2014, NanoMegas), Dr. Alexandros Lappas (June-July 2014, Foundation for Research and Technology - Hellas (FORTH)), Dr. Oleg Prymak (April 2014, U. of Duisburg-Essen), Ms., Kateryna Loza (April 2014, U. of Duisburg-Essen), Dr. Mouath Shatnawi (Aug-Oct 2013, Hashemite U., Jordan), Miss Dragica Podgorski (March - June 2012, U. Frankfurt), Yung-Jin (Joey) Hu (June 2012, Argonne Natl. Lab.), Miss Dragica Podgorski (November 2012, U. Frankfurt), Mr. Daniel Tordari (July 2011, U. Valencia), Dr. Mouath Shatnawi (June-Dec 2011, Hashemite U., Jordan), Ms. Kirsten Jensen (Jan-June 2011, U. Aarhus), Dr. Il-Kyong Jeong (June 2010, U. Puhan, Korea), Ms. Sabrina Disch (Sept. 2008), Dr. Monica Dapiaggi, (Sept-October 2006, U. Milan), Dr. Lorenzo Malavasi (Fall 2005), Dr. F. Atassi (summer 2005, Purdue U), Prof. Sang-Wook Han (Jan 2004), Mr. Gaetano Campi (2002-03), Prof. Jean Chung (2002), Prof. Jean Chung (2001), Dr. O. Stachs (1999), Prof. A. R. Day (1999), Dr. Vicki Nield (1997), Dr. Sidhartha Pattanaik (1997), Dr. Ariane Eberhardt (1997), Dr. Rick Jacubinas (1996), Mr. Michael Kane (1995).

### **Undergraduate and high school students carrying out research in the lab.**

Daniel Puttnam, Carlos Martin, Derek Tropf, Justin Calamari, Adam Jaffe, Xian Yang, Erica Yee (all Columbia, 2015-16), Sarah Stone (Brooklyn Institute of Technology 2015), Karim Mukaddem (Columbia, 2014). Kang (Columbia 2014), Eric Borzuk (Columbia, 2014), Youbin Kim (Stuyvesant High School, 2013), Zane Friedman (Bard High School and Early College, 2013), Michael Salzman (Columbia 2013), Richard “Rusty” Roberts (Columbia 2013-2014), Cole Stephens (Columbia, 2013-2014), Valentina Felsen (York College Undergrad, RPU program 2011), Amir Mazaheripour (Columbia Undergrad, RPU program 2010), John Hong (Bronx High School of Science, NY 2009-2011), Margaret Shaw (North Hunterdon High School, NJ, 2007), Rick Worhatch (MSU undergrad 2005-2006), Dan Lash (MSU undergrad 2005-2006) Kim Venta (MSU undergrad 2006) Dan O'Brien (MSU undergrad 2006), Curtis Walkons (MSU undergrad 2006), Adam DeConink (MSU undergrad, 2005)

### **Past and current research grants [through 2011]**

#### ***External research grants***

<b>Total External Funding</b> (All grants, not including pending)	<b>\$50,757,368</b>
<b>Total External Funding</b> (Grant income to home institution, not	<b>\$26,787,136</b>

	including pending)		
	<b>Total External</b>		
	<b>Funding</b> (S.J.B. amount, not including pending)		<b>\$5,565,948</b>
Use of Pair Distribution Function Analysis to determine the Surface Energy of Nanoparticle Catalysts	<b>Toyota Corporation and Georgia Institute of Technology</b>	<b>\$20,228</b>	09/01/10-08/31/11
Re-Defining Photovoltaic Efficiency Through Molecule Scale Control	<b>DOE-EFRC</b> (with 19 other PIs)	<b>\$15,254,325</b> (SJB amount ~\$200,000)	09/01/09-08/31/14
Pair Distribution Function (PDF) 2010 Study to Characterise Pharmaceutical Amorphous Compounds	<b>GlaxoSmithKline</b>	<b>\$26,000</b>	09/01/10-08/31/11
FRG: Beyond Crystallography: Structure of Nanostructured Materials	<b>NSF-DMR</b> (PI with CoPIs C-Y. Ruan, M. G. Kanatzidis, M. F. Thorpe)	<b>\$1,000,000</b> <b>\$520,000</b> (SJB and C-Y Ruan amt)	08/01/07-07/31/11
Detector for new Rapid Acquisition PDF beam-line development at NSLS (Supplement to DOE-BES grant below)	<b>DOE-BES</b>	<b>\$279,894</b>	6/1/06-5/31/07
Distributed Data Analysis for Neutron Scattering Experiments (Construction proposal)	<b>NSF-IMR-MIP</b> (lead PI's Brent Fultz, Michael Aivazis)	<b>\$11,973,270 M</b> (SJB amt ~\$1.43 M)	8/1/05-7/31/10
Nanostructure determination by co-refining models to multiple datasets	<b>DOE-BES</b> (PI with Co-PI P. M. Duxbury)	<b>\$288,195</b>	9/1/04 – 5/31/08
Distributed Data Analysis for Neutron Scattering Experiments (Design proposal)	<b>NSF-IMR-MIP</b> (lead PI's Brent Fultz, Michael Aivazis )	<b>\$985,414</b> (SJB amt \$121,295)	9/1/04 – 8/31/05
Structure of nanocrystals	<b>NSF-NIRT</b> (PI with Co-PI's Valeri Petkov, M. G. Kanatzidis and M. F. Thorpe)	<b>\$1,350,000</b> (SJB amt \$596,567)	08/03-07/08
Development of medium resolution inelastic x-ray scattering (MERIX) spectrometer for the study of correlated electron systems	<b>DOE-ANL</b>	<b>\$109,670</b>	8/16/02 – 8/15/07
Disordered oxidic and non-oxidic mesostructures	<b>NSF-CHE</b> (Co-PI with PI T. J. Pinnavaia, and Co-PI's M. G. Kanatzidis, M. F. Thorpe, S. D. Mahanti and T. Hogan)	<b>\$2,232,644</b> (SJB amt. ~\$300,000)	07/02-07/05
Local atomic structure of functional materials using pair distribution function analysis of neutron and x-ray data	<b>DOE-BES</b>	<b>\$330,000</b> (with Thorpe; sjb amt \$210,000)	09/01 – 08/04
Local Structure-Property relationship of electronic oxides (funds a post-doc at ISIS)	<b>DOE-BES</b>	<b>\$200,000</b>	1/01-1/03
Probing the Electronic State of Novel Materials using the Local	<b>NSF-DMR</b>	<b>\$330,000</b>	7/00-6/03

## Atomic Structure

Charge Inhomogeneities on Different Length-scales probed with high-resolution neutron diffraction	<b>CRDF</b> -cooperative grant program (with A. Balagurov Joint Institute of Neutron Research and E. Antipov, Moscow State University)	<b>\$50,000</b> (SJB amount \$7167)	10/1/00 - 3/31/02
Neutron Scattering Studies of Structure and Dynamics in Disordered Mesoporous Materials	<b>USDC-NIST</b> (with Pinnavaia)	<b>\$155,030</b> (SJB amount 155,030)	7/99-6/01
Disordered inorganic nanostructures	<b>NSF-CHE</b> (with Kanatzidis, Mahanti, Pinnavaia and Thorpe)	<b>\$1,917,858</b> (SJB amount ~\$200,000)	7/99-6/02
Local atomic structure and properties of transition metal oxides using pair distribution function analysis	<b>NSF-DMR</b> 9700966	<b>\$270,000</b>	8/97-7/00
Local atomic structure of semiconductor alloys using pair distribution function analysis	<b>DOE-BES</b> DE-FG02-97ER45651 (with Thorpe)	<b>\$431,395</b>	8/97-7/01
Electronic and structural properties of colossal magnetoresistant oxides	<b>NSF-MRSEC</b> seed research grant	<b>\$66,000</b> (with Rong Liu; SJB amt:\$22,500)	1/97 - 1/99
Disordered and lower-dimensional porous materials	<b>NSF CHE</b> -9633798 (with Kanatzidis, Mahanti, Pinnavaia and Thorpe)	<b>\$1,760,865</b> ; SJB amount:\$120,000	8/96 - 8/99
A study of the local structure of transition metal oxides using pair distribution function analysis	<b>DOE-LANL</b> subcontract	<b>\$210,000</b>	8/96 - 8/98
no title	<b>Alfred P Sloan Research Fellowship</b>	<b>\$30,000</b>	12/15/95 - 12/15/97

## *University research grants*

Nanoscale Inhomogenieties in Novel Electronic Materials	CFMR (with S. Tessmer, S. D. Mahanti and M. Kanatzidis)	\$40,000 (SJB amt \$16.5k)	8/03-7/04
Cluster Refinement Method for PDF Analysis: Application to Cuprates and Manganites	CFMR (with P. M. Duxbury)	\$20,000	8/01-7/02
Modeling molecular structure in the atomic pair distribution function	CFMR (with M. F. Thorpe)	\$28,000	8/01-7/02
Stability and lattice dynamics of delta plutonium	CFMR (with M.F. Thorpe)	\$26,000	8/00-7/01
Atomic resolution of local structure in semiconductor alloys	CFMR (with M.F. Thorpe)	\$10,000	8/99-7/00
Modelling defects in topologically connected networks: Application to perovskite structures	CFMR (with M.F. Thope)	\$13,000	6/98-6/99
Theoretical and Experimental studies of electronic and structural properties of pristine and doped manganites	CFMR(with J. Harrison, T. Kaplan and S.D. Mahanti)	\$33,000; SJB amt: \$13,000	6/98-6/99

Local atomic structure of semiconductor alloys using pair distribution function analysis	CFMR (with M.F. Thope)	\$13,000	6/97 - 6/98
Electronic and magnetic structure of transition metal oxides and related systems	CFMR (with J. Harrison, Kaplan and Mahanti)	\$45,000; SJB amt: \$23,000	6/97 - 6/98
Disordered and lower dimensional porous materials	CFMR (with Kanatzidis, Mahanti, Pinnavaia and Thorpe)	\$65,000; SJB amt: \$0	6/97 - 6/98
Local atomic structure of semiconductor alloys using pair distribution function analysis	CFMR	\$13,000	6/96 - 6/97
Electronic and magnetic structure of transition metal oxides and related systems	CFMR (with J. Harrison, Kaplan and Mahanti)	\$45,000; SJB amt: \$23,000	6/96 - 6/97
Disordered and lower dimensional porous materials	CFMR (with Kanatzidis, Mahanti, Pinnavaia and Thorpe)	\$65,000; SJB amt: \$0	6/96 - 6/97
Local atomic structure of small clusters in host lattices	AURIG	\$15,000	5/95 - 8/96
Local structure and properties of transition metal oxides using pair distribution function analysis	CFMR	\$20,000	6/95 - 6/96
<b>Total Funding (SJB amount)</b>		<b>\$217,000</b>	

### *Equipment grants*

Detector for new Rapid Acquisition PDF beamline development at NSLS	DOE-BES: Mid-Scale Instrumentation	Sole PI	\$250,000	6/07-5/09
Acquisition of State-of-the-Art Detectors for Materials Research at the Advanced Photon Source	NSF: Instrumentation	with A.I. Goldman (Iowa State), M. Winokur (U. Wisconsin, P. Micelli (U. Missouri) and K. Kelton (Washington University, St. Louis)	\$295,000	Pending
Development of the bending magnet beamlines in the MUCAT sector at the APS	DOE-BES	with A.I. Goldman (Iowa State), M. Winokur (U. Wisconsin, P. Micelli (U. Missouri) and K. Kelton (Washington University, St. Louis)	\$1,200,000	9/00-8/03
High-intensity, high-Q, high-resolution powder diffraction (H <sup>3</sup> PD)	NSF-instrumentation	Co-PI's: T. Egami (U. Penn) S.J.L. Billinge with 4 others	\$800,000	9/00-8/02
Wide angle capability for the high-resolution chopper spectrometer PHAROS at Los Alamos	DOE: Energy research financial assistance program	with Robinson, Aranson, Broholm, Eckert and Egami	\$536,000	funded 1996

### **Collaboration memberships and facilities construction projects**



1. **Powder Instrument Next Generation (PING).** I am spokesperson for the Beamline Advisory Team (BAT) for the powder diffraction and PDF beamlines that will be constructed as part of the construction project for NSLS-II at Brookhaven National Laboratory. Expected completion is 2015.
2. **PDF beamline development at the National Synchrotron Light Source (NSLS) beam-port X17A.** Co leading (with Lars Ehm, SUNY-Stony Brook) the development of a PDF beamline development at NSLS, to be constructed in 2009-2010.
3. **High-intensity, high-Q, high-resolution powder diffraction (H<sup>3</sup>PD) instrument for the LANSCE beamline** Collaboration (T. Egami and S. J. L. Billinge spokespeople, also including 4 other researchers from Academia) to build a neutron powder diffractometer at Los Alamos for materials science and the study of complex materials using Rietveld and PDF methods (see NSF instrumentation grant, above). Diffractometer is now called NPDF and was constructed on time and under budget. It has entered the Manuel Lujan, jr., Neutron Scattering Center user program. It is currently the highest resolution and highest data-rate (5-times faster than SEPD at IPNS) powder diffractometer at a spallation source in the US.
4. **Mid-West Universities Collaborative Access Team:** Collaboration to build and operate an x-ray beamline at the Advanced Photon Source at Argonne National Laboratory for local structure studies of complex materials (see DOE-BES grant above). I am lead Co-PI with Prof. Alan Goldman on this project. The hutches and upstream beam transport components are in place. The optics and beam-line components are ordered and detailed designs are in place. The objective is to make a beamline that is stable and easy to use for high-resolution PDF studies. Two ID beamlines and three experimental stations are already built and operated by the CAT, that includes researchers from 8 Universities, for surface studies under high vacuum conditions, magnetic scattering and high energy diffraction.
5. **Collaboration to build a wide angle capability for the high-resolution chopper spectrometer PHAROS at Los Alamos:** with R.A. Robinson (LANL), M. Aranson (U. Michigan), C. Broholm, J. Eckert (LANL) and T. Egami (U. Penn). This project was funded and the Pharos upgrade has been carried out at LANSCE. My involvement in this project was peripheral.

## 6. Publications

### *Patents*

1. Simon J. L. Billinge, **Systems and Methods for Educational Social Networking**, *Patent Pending* (2013).
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### **Invited talks**

1. S. J. L. Billinge, **Light Sources for Materials and the aFLS context**, *Keynote at the 1st African Light Source Conference and Workshop Grenoble France*, November 17th (2015).
2. S. J. L. Billinge, **The Materials Complexity Frontier: nanostructure and heterogeneities**, *Workshop "Pair Distribution Function Analysis: The local point of view of material development" Diamond Light Source Rutherford Appleton Laboratory Oxfordshire UK*, September 2nd-3rd (2015).
3. S. J. L. Billinge, **The Materials Complexity Frontier: nanostructure and heterogeneities**, *Workshop "Pair Distribution Function Analysis: The local point of view of material development" Diamond Light Source Rutherford Appleton Laboratory Oxfordshire UK*, September 2nd-3rd (2015).
4. S. J. L. Billinge, **Structure of nanomaterials using PDF and ePDF methods**, *2015 European Crystallography Meeting (ECM2015) Croatia*, August 24th (2015).



5. S. J. L. Billinge, **Robust prediction of real materials**, *2015 New York Scientific Data Summit New York NY*, August 2nd - 5th (2015).
6. S. J. L. Billinge, **Amorphous or nanocrystalline? Advances in the total scattering pair distribution function methods for characterizing amorphous and nanocrystalline pharmaceuticals**, *Powder Pair Distribution Function and Pharmaceuticals session of the 2015 American Crystallographic Association Annual Meeting Philadelphia PA*, July 25th - 29th (2015).
7. S. J. L. Billinge, **Teaching an old dog new tricks: new opportunities in amorphous- and nano-structure determination by combining the venerable PDF method with modern experimental sources**, *22nd International Symposium on Metastable Amorphous and Nanostructured Materials (ISMANAM15) Paris France*, July 13th - 17th (2015).
8. S. J. L. Billinge, **Nanoscale fluctuations in electronic and atomic structure in strongly correlated electron and charge ordered systems**, *Superstripes 2015: Quantum in Complex Matter: Superconductivity Magnetism and Ferroelectricity Ischia Italy*, June 14th - 18th (2015).
9. S. J. L. Billinge, **The Debye equation in action: some scientific PDF case-studies powered by the Debye Equation**, *100 Years of the debye scattering equation (DSE2015) Cavalese Trentino Italy*, June 14th - 16th (2015).
10. S. J. L. Billinge, **Amorphous or nanocrystalline? Advances in the total scattering pair distribution function methods for characterizing amorphous and nanocrystalline pharmaceuticals**, *Preclinical Form and Formulation in Drug Discovery Gordon Research Conference Waterville Valley NH*, June 7th - 12th (2015).
11. S. J. L. Billinge, **Nanoscale fluctuations in strongly correlated electron systems**, *Frontiers in Condensed Matter Physics lecture at the 4th Super-PIRE REIMEI Workshop on Frontiers of Condensed Matter Physics Triumpf facility Vancouver Canada*, May 15th - 22nd (2015).
12. S. J. L. Billinge, **Robust Modeling of Real Materials**, *Frontiers in Data Modeling and Simulation Argonne National Laboratory Chicago IL*, March 30th (2015).
13. S. J. L. Billinge, **The Materials Complexity Frontier: Applied Math and Computational Challenges**, *Opportunities in Materials Informatics Madison Wisconsin*, February 9th to 10th (2015).
14. Benjamin A. Frandsen and Simon J. L. Billinge, **Magnetic pair distribution function analysis: introduction and applications**, *American Conference on Neutron Scattering Knoxville TN*, June 1st - 5th (2014).
15. S. J. L. Billinge, **Nanostructure Complex Modeling**, *Supercomputing 2014 (SC14) New Orleans LO*, November 16th - 21st (2014).
16. S. J. L. Billinge, **Total scattering atomic pair distribution function analysis: Theory and methodology**, *High resolution X-ray powder diffraction at the Taiwanese synchrotron (NSRRC) Taipei Taiwan*, October 8th - 9th (2014).
17. S. J. L. Billinge, **The Materials Complexity Frontier: Applied Math and Computational Challenges**, *Smoky Mountains Computational Sciences and Engineering Conference (SMC2014) Gatlinburg TN*, September 2nd - 4th (2014).
18. S. J. L. Billinge, **Search for hidden broken local symmetry states in correlated electron systems**, *The first Nanostructure in the City Symposium Columbia University New York NY*, August 18th (2014).
19. S. J. L. Billinge, **Search for hidden broken local symmetry states in correlated electron systems**, *Superstripes Conference Erice Italy*, July 25th - 31st (2014).
20. S. J. L. Billinge, **Studying competition disorder and nanoscale fluctuations in strongly correlated systems and the necessity of combining methods such as muons x-rays and neutrons**, *Transformative Hadron Beamlines Workshop Brookhaven National Laboratory*, July 21st - 23rd (2014).
21. S. J. L. Billinge, **Amorphous or nanocrystalline? Looking beyond the amorphous halo with the total scattering pair distribution function method**, *Advanced materials and pharmaceutical technologies Polytech Engineering School University of Lille 1 Sciences and Technologies Villeneuve-d'Ascq France.*,

July 9-10th (2014).

22. S. J. L. Billinge, **Atomic structure at the nanoscale: from fuel cells to pharmaceuticals**, *Center for Fundamental Nanomaterials Colloquium Brookhaven National Laboratory Upton New York* , June 10th (2014).
23. S. J. L. Billinge, **Developments in Nanostructure Solution from PDF data**, *American Crystallographic Association Annual Meeting Albuquerque NM* , May 24th - 28th (2014).
24. S. J. L. Billinge, **Atomic structure at the nanoscale: from fuel cells to pharmaceuticals**, *Colloquium National Autonomous University of Mexico Mexico City Mexico* , May 7th (2014).
25. S. J. L. Billinge, **Nanocrystallography: Crystallography for 21st century problems**, *The Seventh National Congress of the Mexican Society of Crystallography (SMCr) Villahermosa Tabasco Mexico* , May 4th - 9th (2014).
26. S. J. L. Billinge, **Search for hidden broken local symmetry states in correlated electron systems**, *Correlated Oxides and Oxide Interfaces Meeting of the William I. Fine Theoretical Physics Institute Minneapolis Minnesota* , May 1st - May 4th (2014).
27. S. J. L. Billinge, **Local dimers and the metal insulator transition in Cu(IrCr)2S4 from PDF and MuSR studies**, *The 3rd Super-PIRE REIMEI Workshop on Frontiers of Condensed Matter Physics Institute of Physics Beijing China* , March 16th - 21st (2014).
28. S. J. L. Billinge, **The Materials Complexity Frontier: nanostructure and heterogeneities**, *Southern African Powder Diffraction Conference and Workshop University of the Witwatersrand Johannesburg South Africa* , January 27th - February 1st (2014).
29. S. J. L. Billinge, **The total scattering atomic pair distribution function analysis method: PDF studies of complex materials**, *Southern African Powder Diffraction Conference and Workshop University of the Witwatersrand Johannesburg South Africa* , January 27th - February 1st (2014).
30. S. J. L. Billinge, **The Materials Complexity Frontier: nanostructure and heterogeneities**, *10th Aarhus Winter Meeting of the Danish Chemical Society University of Aarhus Denmark* , January 24th (2014).
31. S. J. L. Billinge, **Seeing atomic arrangements at the nanoscale: from fuel cells to pharmaceuticals and the African context**, *African Materials Research Society biennial meeting Addis Ababa Ethiopia* , December 12th (2013).
32. S. J. L. Billinge, **Overview of JUAMI**, *JUAMI one year later: Past accomplishments and future prospects special JUAMI symposium at the African-MRS Addis Ababa Ethiopia* , December 10th (2013).
33. S. J. L. Billinge, **Quantitative characterization of multiscale structural complexity in batteries fuel cell and thermoelectric materials using advanced scattering probes**, *Materials Research Society Fall Meeting Boston MA* , December 1st - 6th (2013).
34. S. J. L. Billinge, **Atomic pair distribution function and total scattering studies: Looking at materials on the nanoscale**, *DESY Hamburg* , September 12th - 13th (2013).
35. S. J. L. Billinge, **Complex Modeling: towards more robust nanostructure refinements**, *Workshop Advanced Analysis of X-Ray and Neutron Scattering Data: Getting from data to science Brookhaven National Laboratory Upton NY* , August 14th - 15th (2013).
36. S. J. L. Billinge, **A few words about software for XPD**, *NSLS-II First-Experiments Workshop Brookhaven National Laboratory Upton NY* , August 12th - 13th (2013).
37. S. J. L. Billinge, **Nanoscale disorder stripes and metal insulator transitions: The local structural landscape**, *Quantum in Complex Matter: Superconductivity Magnetism and Ferroelectricity International Conference Superstripes 2013 Rome Italy* , May 27th - June 1st (2013).
38. S. J. L. Billinge, **Complex Modeling: towards more robust nanostructure refinements**, *Accuracy in Powder Diffraction IV (APD-IV) National Institute of Standards and Technology Gaithersburg MD* , April 22nd - 24th (2013).
39. S. J. L. Billinge, **Seeing atomic arrangements at the nanoscale: from fuel cells to**

- pharmaceuticals**, *Launch meeting of the Materials Research Institute Queen Mary College London UK* , April 15th (2013).
40. S. J. L. Billinge, **Emergent nanoscale fluctuations in rock-salt PbTe**, *American Physical Society March Meeting Baltimore MD* , March 18th - 22nd (2013).
  41. S. J. L. Billinge, **Complex Modeling: towards robust solutions to ill-posed inverse problems in scattering**, *Workshop on Computational Scattering Science California Institute of Technology CA* , January 31- February 2nd (2013).
  42. S. J. L. Billinge, **Local structure in complex materials from advanced scattering and computation**, *Joint US-Africa Materials Institute first school on Materials for Sustainable Energy Addis Ababa Ethiopia* , December 10th-21st (2012).
  43. S. J. L. Billinge, **Materials Characterization**, *Joint US-Africa Materials Institute first school on Materials for Sustainable Energy Addis Ababa Ethiopia* , December 10th-21st (2012).
  44. S. J. L. Billinge, **Competition and nanoscale fluctuations in complex materials**, *DOE BES x-ray scattering contractors' meeting* , November 8th-10th (2012).
  45. S. J. L. Billinge, **PDF and total scattering studies: Looking at materials on the nanoscale**, *13th European Powder Diffraction Conference EPDIC 13 Grenoble France* , October 28th-31st (2012).
  46. S. J. L. Billinge, **Life beyond PDFgui: PDFgetX3 SrFit and SrReal. From raw data to flexible Complex Modeling of atomic pair distribution function total scattering data.**, *Lachlan's Software Fayre 13th European Powder Diffraction Conference EPDIC 13 Grenoble France* , October 28th-31st (2012).
  47. S. J. L. Billinge, **Complex Materials Complicated Structures Complex Modeling**, *Advanced Simulation Techniques for Total Scattering Data Los Alamos National Laboratory* , October 16th-19th (2012).
  48. S. J. L. Billinge, **PDFgui/PDFfit2: Small box modeling**, *The first 24 years of Reverse Monte Carlo Modelling Budapest Hungary* , September 20th-22nd (2012).
  49. S. J. L. Billinge, **I. Structure of disordered and nanomaterials II. OK so you decided PDF/Total Scattering may help what next?**, *Scattering methods for the analysis of the structure of matter summer school of the International Max Planck Research School for Advanced Materials Stuttgart Germany* , September 17th-20th (2012).
  50. S. J. L. Billinge, **x-ray and neutron studies of nanoscale structural fluctuations in electronic materials**, *Phase Separation and superstripes in high temperature superconductors and related materials SUPERSTRIPES (2012) Erice Italy* , July 11th-17th (2012).
  51. S. J. L. Billinge, **(1) Overview of local structure and properties of complex materials as studied using total scattering and PDF analysis (2) Introduction to the PDF method including recent developments in data analysis and modeling (3) Case study: pharmaceuticals + hands on demo of modeling the PDF if there is time.** , *Ph.D visiting lecture series at University of Milan Milan Italy* , July 9th-10th (2012).
  52. S. J. L. Billinge, , *Annual 2012 TMS meeting in Orlando FL* , March 11-15 (2012).
  53. S. J. L. Billinge, **Nanostructure - from energy materials to pharmaceuticals**, *Zing Nanoscience Conference Lanzarote Spain* , February 14-17 (2012).
  54. S. J. L. Billinge, **Structure of nanostructured materials using PDF methods at the ESRF and beyond**, *ESRF Users' meeting ESRF Grenoble France* , February 7-8 (2012).
  55. S. J. L. Billinge, **Nanostructure from energy materials to pharmaceuticals: total scattering and the atomic pair distribution function method**, *two-day workshop on the applications of the NYU Bruker GADDS instrument NYU New York* , June 15-16 (2011).
  56. C. L. Farrow and Simon J. L. Billinge, **Complexing the Atomic Pair Distribution Function and Small Angle Scattering for Determining the Structure of Nanoparticles: Challenges and Prospects** , *IUCr Conference 2011 Madrid Spain* , August 22 - 30 (2011).
  57. C. L. Farrow and Simon J. L. Billinge, **The structure of nanoparticles with the atomic pair distribution**

- function**, *Nanoscience Conference 2011* , February 19 - 22 postponed (2011).
58. S. J. L. Billinge, **Nanostructure and Diffraction of Heterogeneous Materials with Nanobeams**, *Workshop on Materials Science with Coherent Nanobeams at the Edge of Feasibility at Cornell University* , June 27-28 (2011).
  59. S. J. L. Billinge, **Software Enabling Science: Nanostructure from diffraction**, *American Crystallographic Association annual meeting New Orleans LA* , May 28th - June 2nd (2011).
  60. S. J. L. Billinge, **Material structure in the nano-world: The nanostructure problem and modern scattering methods for solving it** , *Gordon Research Conference on Clusters Nanocrystals & Nanostructures Mount Holyoke College in South Hadley MA* , July 24th - 29th (2011).
  61. S. J. L. Billinge, **Complicated problems: complex materials and complex modeling** , *Workshop on the analysis of diffraction data in real-space (ADD2011) ESRF Grenoble* , October 11th - 14th (2011).
  62. S. J. L. Billinge, **Total Scattering Pair Distribution Functions (TSPDF) for Fingerprinting Amorphous Pharmaceuticals**, *10th Pharmaceutical Powder X-ray Diffraction Symposium (PPXRD-10) Lyon France* , May 16th - 19th (2011).
  63. S. J. L. Billinge, **Software Products from the DANSE Diffraction Subgroup**, *Last DANSE Conference Workshop Caltech Pasadena CA* , May 4th - 6th (2011).
  64. S. J. L. Billinge, **Material structure in the nano-world: The nanostructure problem and modern scattering methods for solving it** , *International Conference on Communication Computational skills and Nanotechnology Swami Ramanand Teerth Marathwada University Nanded Maharashtra State India* , January 11th - 13th (2011).
  65. Emil S. Bozin, Ahmad S. Masadeh, Yew S. Hor, John F. Mitchell and Simon J.L. Billinge , **Local structural aspects of the metal-insulator transition in CuIr<sub>2</sub>S<sub>4</sub> from total scattering x-ray study**, *EPDIC12 12th European Powder Diffraction Conference Darmstadt Germany* , August 27-31 (2010).
  66. S. J. L. Billinge, **Structure at the Nanoscale: atomic pair distribution function analysis of nanostructured materials**, *J. D. Hanawalt prize session of the Denver X-ray Conference Denver CO* , August 2nd - 6th 2010 (2010).
  67. S. J. L. Billinge, **Pair Distribution Function Technique: Principles and Methods**, *Diffraction at the Nanoscale: Nanocrystals Defective and Amorphous Materials Paul Scherrer Institute Villigen Switzerland* , May 24th-30th (2010).
  68. S. J. L. Billinge, **Structure at the Nanoscale: atomic pair distribution function analysis of nanostructured materials**, *British Crystallographic Association Annual Meeting University of Warwick Warwick UK* , April 12th - 15th (2010).
  69. S. J. L. Billinge, **Characterising nanoscale molecular packing: Data and modeling**, *CPOSS annual meeting University College London UK* , April 19th (2010).
  70. S. J. L. Billinge, **The atomic pair distribution function (PDF) method for studying amorphous and nanocrystalline materials**, *Amorphous III Conference - Multi-component amorphous materials formulation processing and stability meeting of the Academy of Pharmaceutical Sciences University of Nottingham UK* , April 21st (2010).
  71. S. J. L. Billinge, **Material structure in the nano-world: The nanostructure problem and modern scattering methods for solving it**, *2009 Advances in X-Ray Scattering & Diffraction Workshop Delta Guelph Hotel and Conference Centre in Guelph Ontario* , October 26th (2009).
  72. S. J. L. Billinge, **The importance of local structure in functional materials from atomic pair distribution function analysis measurements** , *Local distortions and Physics of Functional materials (LPF09) Frascati Italy* , July 22nd - 24th (2009).
  73. S. J. L. Billinge, **Recent developments in atomic pair distribution function analysis applied to amorphous and nanocrystalline materials**, *Applications of Synchrotron Techniques in Glass Research Brookhaven National Laboratory* , April 6th - 7th (2009).

74. S. J. L. Billinge, **Atomic pair distribution function (PDF) analysis for the study of structure at the nanoscale**, *10th international school and workshop of crystallography of the Egyptian society of crystallography and its applications (ESCA) Ain Soukhna Egypt* , February 1st - 5th (2009).
75. S. J. L. Billinge, **Atomic pair distribution function (PDF) analysis hands-on tutorials PDFgetX2 and PDFgui**, *10th international school and workshop of crystallography of the Egyptian society of crystallography and its applications (ESCA) Ain Soukhna Egypt* , February 1st - 5th (2009).
76. S. J. L. Billinge, **DiffDANSE 2008 report**, *DANSE developers meeting California Institute of Technology Pasadena CA* , January 26th-28th (2009).
77. S. J. L. Billinge, **Material structure in the nano-world: The nanostructure problem and our efforts at solving it**, *invited talk iNANO 7th Annual meeting Aarhus Denmark* , January 21st (2009).
78. S. J. L. Billinge, **atomic pair distribution function analysis**, *invited talk Analytical approaches workshop Center for Green Materials Chemistry U. Oregon Eugene OR* , January 12th (2009).
79. S. J. L. Billinge, **The nanostructure problem: Solving the inverse problem for nanostructure from scattering data**, *invited talk 21st International CODATA Conference "Scientific information for society - form today to the future"* , October 1st - 4th (2008).
80. S. J. L. Billinge, , *Inter-American Materials Collaboration (CIAM) symposium Guarujá near São Paulo Brazil* , September 29th - October 2nd (2008).
81. S. J. L. Billinge, **FRG grant Overview and summary of activities in the Billinge group**, *Beyond crystallography: Structure of nanostructured materials Tempe AZ* , May 17 - May 20 (2008).
82. S. J. L. Billinge, **Nanostructure refinement and solution** , *XXI Congress and General Assembly of the International Union of Crystallography Osaka Japan* , August 23-31 (2008).
83. C. L. Farrow, C.-Y. Ruan and S. J. L. Billinge, **Extracting quantitative structural parameters from ultrafast electron crystallography**, *Beyond crystallography: Structure of nanostructured materials Tempe AZ* , May 17 - May 20 (2008).
84. S. J. L. Billinge, **TBD** , *Complex and nanostructured materials for energy applications Michigan State University East Lansing MI* , June 22nd - 26th (2008).
85. S. J. L. Billinge, **Neutrons for structural determination** , *Advances in Neutron Scattering APS March meeting workshop New Orleans* , March 9th (2008).
86. S. J. L. Billinge, **Nanostructure refinement and solution from high energy diffraction data** , *annual meeting of the German Crystallographic Society (DGK2008) University of Erlangen Germany* , March 3-6 (2008).
87. S. J. L. Billinge, **Nanostructure refinement and solution from the atomic pair distribution function (PDF)**, *Workshop on Local Structure Measurements NIST Gaithersburg MD* , February 20-21 (2008).
88. S. J. L. Billinge, **Local Structure-Property relationships in Strongly Correlated Electron Materials and Beyond**, *Workshop on Hard Condensed Matter and Materials Physics at NSLS-II Brookhaven National Laboratory Upton NY* , February 5-6 (2008).
89. S. J. L. Billinge, **Total scattering and atomic pair distribution function (PDF) methods: overview** , *ICMR-JNCASR Winter School in Bangalore India* , December 6 - December 13 (2007).
90. S. J. L. Billinge, **Total scattering and atomic pair distribution function (PDF) methods: theory and practice** , *ICMR-JNCASR Winter School in Bangalore India* , December 6 - December 13 (2007).
91. S. J. L. Billinge, **The nanostructure problem: how can we get quantitative 3D structures from nanomaterials?**, *Bangalore Nano 2007 meeting Bangalore India* , December 6 - December 7 (2007).
92. S. J. L. Billinge, **Structure solution and refinement of nanostructures from atomic pair distribution function data** , *Workshop on PDF on the nanoscale European Synchrotron Radiation Facility 2007. Grenoble (France)* , 22nd - 23rd October (2007).
93. S. J. L. Billinge, **Pair distribution function approach for characterization of nanocrystals** , *5th Size-*

*Strain Conference - Diffraction Analysis of the Microstructure of Materials Garmisch-Partenkirchen (Germany)*, 7th-9th October (2007).

94. S. J. L. Billinge, **Local structures from powders: recent advances in atomic pair distribution function methods and modeling** , *Diffuse Scattering for the Masses: Local Structural Correlations in Molecular Macromolecular and Inorganic Crystals Transactions symposium of the American Crystallographic Association annual meeting Salt Lake City UT.* , July 21st - 26th (2007).
95. S. J. L. Billinge, **TBA** , *Structure and Dynamics in Soft Matter and Macromolecules: from Single Molecules to Ensembles ICTP Trieste Italy* , 4th-8th June (2007).
96. S. J. L. Billinge, **The Nanostructure Problem: structure of complex nanostructured materials** , *Latin American Workshop on Applications of Powder Diffraction Campinas Brazil* , 18th-20th April (2007).
97. S. J. L. Billinge, **The Atomic Pair Distribution Function Method** , *Workshop on Methods of Powder Diffraction satellite to Latin American Workshop on Applications of Powder Diffraction* , 16th-17th April (2007).
98. S. J. L. Billinge, **Structure studies of nanostructured energy related materials** , *MRS Symposium JJ: Functional Nanoscale Ceramics for Energy Systems San Francisco California* , 9th-13th April (2007).
99. S. J. L. Billinge, **The nanostructure problem** , *Hume-Rothery Symposium on Scattering Studies and the Fundamental Properties of Materials TMS spring meeting Orlando FL* , 25th February - 1st March (2007).
100. S. J. L. Billinge, **Total scattering: overview** , *Recent Developments in Nanomaterials Joint ICTP and ICMR workshop Trieste Italy* , 15th - 19th January (2007).
101. S. J. L. Billinge, **Total Scattering: theory** , *Recent Developments in Nanomaterials Joint ICTP and ICMR workshop Trieste Italy* , 15th - 19th January (2007).
102. S. J. L. Billinge, **Studies of nanostructure using neutron total scattering analysis** , *The US-China Workshop Series on Neutron Scattering Science and Technology Beijing China* , November 12-15 (2006).
103. S. J. L. Billinge, **Real Space Rietveld and other PDF profile refinement strategies** , *RMC-3: The First 18 Years of Reverse Monte Carlo Modelling Budapest Hungary* , 28th-30th September (2006).
104. S. J. L. Billinge, **Atomic pair distribution function (PDF) analysis of x-ray powder diffraction to study nanostructured materials** , *workshop on X-ray analysis of nanostructures Geneva Switzerland* , 31 August (2006).
105. S. J. L. Billinge, **The nanostructure problem and some first steps to solve it** , *Plenary lecture at the 10th European Powder Diffraction Conference Geneva Switzerland* , 1-4th September (2006).
106. S. J. L. Billinge, **Combined crystallographic methods for the ab-initio solution of the nanostructure problem** , *Synchrotron Radiation for Materials Science Chicago IL* , 30 July - 2 August (2006).
107. S. J. L. Billinge, **The nanostructure problem** , *Gordon Research Conference on Solid State Chemistry* , 23-28 July (2006).
108. S. J. L. Billinge, **The nanostructure problem: what is it why do we care and what are we doing about it?** , *Symposium in honor of George H. Kwei Los Alamos NM* , 28-30 June (2006).
109. S. J. L. Billinge, **Novel electronic materials studied on NPDF** , *BES review of LANSCE Los Alamos National Laboratory* , 21 March (2006).
110. S. J. L. Billinge, **Software and the status of the DANSE project** , *NOMAD instrument IDT meeting Baltimore MD* , 13th March (2006).
111. S. J. L. Billinge, **The nanostructure problem** , *Lansce User Group Meeting Los Alamos National Laboratory* , September 11-13 (2005).
112. S. J. L. Billinge, **Peter Piper picked a problem trickier than most. Can computer science help solve the problem peter piper picked?** , *The XX Congress and General Assembly of the International Union of Crystallography Florence Italy* , August 23-31 (2005).
113. S. J. L. Billinge, **Atomic pair distribution function software** , *Siena Crystallographic Computing School* ,

18th to 23rd August (2005).

- 114.S. J. L. Billinge, **Data processing in preparation for PDF analysis using PDFgetX2**, *Workshop on Structure Solution and Refinement of difficult structures using powder diffraction Orlando FL*, 28th May (2005).
- 115.S. J. L. Billinge, **Advanced scattering methods for solving the atomic-scale structure of nanostructured materials**, *Defects in Nanostructures Conference of the Michigan Chapter of the American Vacuum Society*, May 11 (2005).
- 116.S. J. L. Billinge, **Fast in-situ high-resolution pair distribution function analysis studies of local structure in glasses and nanocrystalline materials**, *American Physical Society March meeting*, 21-25th March (2005).
- 117.S. J. L. Billinge, **Nanoscale structures in complex crystals using Neutron Pair Distribution Function Methods (invited)**, *TMS Annual Meeting in San Francisco*, 13-17 February (2005).
- 118.S. J. L. Billinge, *workshop on Local Structure in Materials and Disorder in Crystalline Materials Oak Ridge TN*, 31st October - 3 November (2004).
- 119.S. J. L. Billinge, **Strain and nanostructure in correlated electronic oxides**, *Nanoscale Heterogeneity and Quantum Phenomena in Complex Matter University of Roma*, 26th September - 2 October (2004).
- 120.S. J. L. Billinge, **Atomic pair distribution function analysis and powder diffraction of nanocrystalline materials**, *European Powder Diffraction Conference*, 2-5 September (2004).
- 121.S. J. L. Billinge, **TBA**, *Science with High-Energy X-Rays August 9-10*, 9-10 August (2004).
- 122.S. J. L. Billinge, **Nanocrystallography: the study of nanostructured materials**, *Flexibility in complex materials: glasses amorphous and proteins Sainte-Adèle Québec (Canada)*, 7-10 August (2004).
- 123.S. J. L. Billinge, **Probing the electronic state of the manganites from the local structure**, *Colossal Magnetoresistive and Related Transition Metal Oxides Telluride Colorado*, 28th June - 5th July (2004).
- 124.S. J. L. Billinge, **PDF workshop**, *2004 American conference of neutron scattering College Park Maryland*, 7-10 June (2004).
- 125.S. J. L. Billinge, **DANSE breakout session**, *2004 American conference of neutron scattering College Park Maryland*, 7-10 June (2004).
- 126.S. J. L. Billinge, **TBA**, *Applications of neutron scattering in chemistry*, 4-6 June (2004).
- 127.S. J. L. Billinge, **Structure of Nanocrystals and Crystallographically Challenged Materials Using Hard X-rays and the Atomic Pair Distribution Function Method**, *2004 NSLS users meeting*, 18 May (2004).
- 128.S. J. L. Billinge, **X-ray pair distribution studies of local structure in disordered crystals nanocrystals and glasses**, *Workshop on x-ray structural studies of containerless processed intermetallic alloys and liquids*, 26-27 February (2004).
- 129.S. J. L. Billinge, **Powder diffractometry and DANSE: powDANSE**, *Data analysis of neutron scattering experiments Caltech Pasadena CA*, 3rd-6th September (2003).
- 130.S. J. L. Billinge, **The charge order orbital order delocalization competition: adding orbital occupancy to the decision making process**, *Self-organized Strongly Correlated Electron Systems Santorini Greece*, 27 to the 30th of August (2003).
- 131.S. J. L. Billinge, **Nanocrystallography: the study of nanostructured materials**, *Annual meeting of the American Crystallographic Association Cincinnati OH USA*, July 26-31 (2003).
- 132.S. J. L. Billinge, **Nanocrystallography: nanoscale ordering starting from crystalline materials**, *Fluctuation Electron Microscopy and Nanoscale Ordering in Amorphous Materials University of Illinois Urbana-Champaign IL USA*, June 23-24 (2003).
- 133.S. J. L. Billinge, **Nanoscale electronic microstructures in correlated electron oxides**, *Dynamic inhomogeneities in complex oxides Bled Slovenia*, June 14-19th (2003).

- 134.S. J. L. Billinge, **Beyond crystallography: the study of disorder nanocrystallinity and crystallographically challenged materials**, *Morley award symposium of the ACS in honor of Mercuri Kanatzidis Cleveland OH*, 4th June (2003).
- 135.S. J. L. Billinge, **Beyond crystallography: the structure of complex and nanocrystalline materials**, *Midwest High Temperature and Solid State Chemistry Conference Michigan State University*, May 29-31 (2003).
- 136.S. J. L. Billinge, **Nanoscale electronic microstructures in correlated metals from neutron PDF measurements**, *International Symposium on Inhomogeneous and Strongly Correlated Materials with Novel Electronic Properties (ISCM) - SMEC2003 Miami (FL USA)*, 24-27 March (2003).
- 137.S. J. L. Billinge, **Glasses and disordered materials: theory and methods**, *Neutrons In solid state Chemistry and the Earth Sciences Today and tomorrow (NICEST) Oak Ridge TN USA*, 12-17 March (2003).
- 138.S. J. L. Billinge, **Nanoscale Electronic Microstructures: Signatures and Consequences**, *Fourth International Conference on New Theories Discoveries and Applications of Superconductors and Related Materials San Diego CA*, Jan 16-21 (2003).
- 139.S. J. L. Billinge, **Complex Materials: Beyond Crystallography the Structural Mean-Field Approximation**, *From Solid State to BioPhysics Cavtat near Dubrovnik in Croatia*, 13-19 June (2002).
- 140.S. J. L. Billinge, **Structural compliance misfit strain and stripe nanostructures in cuprate superconductors**, *Intrinsic Multiscale Structure and Dynamics of Complex Electronic Oxides ICTP Trieste*, 1-4 July (2002).
- 141.S. J. L. Billinge, **Structural compliance misfit strain and stripe nanostructures in cuprate superconductors**, *International conference on superconductivity CMR and related materials: novel trends Giens France*, 1-8 June (2002).
- 142.S. J. L. Billinge, **Species intercalated in zeolites using INS**, *American Conference on Neutron Scattering (ACNS) Knoxville TN*, June 23-27 decl (2002).
- 143.S. J. L. Billinge, **Structural compliance misfit strain and stripe nanostructures in cuprate superconductors**, *Artificial and natural nanostructures MgB and related systems - ANN2001 Roma*, 10-12 December (2001).
- 144.S. J. L. Billinge, **Structural compliance misfit strain and stripe nanostructures in cuprate superconductors**, *Networks and Nanoscale Coherence in 2D Metals and HTSC Banff Canada*, August 22-25th (2001).
- 145.S. J. L. Billinge, **Polarons from powders**, *From Semiconductors to Proteins: Beyond the Average Structure Traverse City Mi*, July 28-August 1st (2001).
- 146.S. J. L. Billinge, **Beyond the average structure: neutron and x-ray studies of complex materials**, *American Crystallographic Association annual meeting Los Angeles*, July 21-26 (2001).
- 147.S. J. L. Billinge, **Local structure and high Tc superconductivity: tilts stripes strain and cigars**, *international workshop MSU-HTSC VI "High temperature superconductors and novel inorganic materials engineering" Moscow-St. Petersburg Russia*, June 24-30th (2001).
- 148.S. J. L. Billinge, **Real space pair distribution functions: the good the bad and the ugly and how can we tell the difference?**, *Accuracy in Powder Diffraction to be held at National Institute of Standards and Technology Gaithersburg MD*, April 22-25th (2001).
- 149.S. J. L. Billinge, **The metal-insulator transition in CMR manganites: a strange kind of percolation**, *APS March meeting Seattle WA*, March 12-16th (2001).
- 150.S. J. L. Billinge, **Microscopic charge inhomogeneities in underdoped cuprates: local structural evidence**, *The Third International Conference on New Theories Discoveries and Applications of Superconductors and Related Materials (New3SC-3) Honolulu Hawaii*, January 15-19 (2001).
- 151.S. J. L. Billinge, **NPD upgrade project: A total scattering powder diffractometer**, *Basic Energy*



- Sciences Advisory Committee subcommittee review of BES operated user facilities Los Alamos National Laboratory* , 14th November (2000).
- 152.S. J. L. Billinge, **Electronic inhomogeneities and properties of complex oxides**, *Basic Energy Sciences Advisory Committee subcommittee review of BES operated user facilities Argonne National Laboratory* , 16th November (2000).
- 153.S. J. L. Billinge, **High resolution total scattering from poorly crystallized materials**, *Disordered Materials Diffractometer Instrument Advisory Team workshop Argonne National Laboratory* , November 19th (2000).
- 154.S. J. L. Billinge, **Structures from Crystallographically Challenged Samples: Taking a Real-Space Approach**, *invited talk at a special session "Pushing the limits of powder diffraction" at the Pittsburgh Diffraction Conference held in Pittsburgh* , 26-28 October (2000).
- 155.S. J. L. Billinge, **Atomic Pair Correlations in Solids**, *American Chemical Society Annual Meeting* , August 20-24 (2000).
- 156.S. J. L. Billinge, **Dynamic charge inhomogeneities in underdoped cuprates from the atomic pair distribution function**, *Stripes 2000 Conference Rome Italy* , September 25-30 (2000).
- 157.S. J. L. Billinge, **The Local Structure-Function relationship in Partially Ordered Materials: The Essential Role of Neutrons**, *American Crystallographic Association annual meeting Minneapolis* , July 22-26 (2000).
- 158.S. J. L. Billinge, **Charge Inhomogeneities and the Metal-Insulator Transitions in the CMR Manganites**, *Telluride Workshop: CMR Manganites and Related Transition Metal Oxides Telluride Colorado* , July 16-21 (2000).
- 159.S. J. L. Billinge, **Microscopic Charge Inhomogeneities and the Pseudo Gap in Underdoped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ : Local Structural Evidence**, *Major Trends in superconductivity in the new millennium Klosters Switzerland* , April 1-6 (2000).
- 160.S. J. L. Billinge, **Short and Intermediate Range Order in Materials Using the Atomic Pair Distribution Function Method**, *XVIIIth International Union of Crystallography congress and General Assembly Glasgow Scotland* , 4th-13th August (1999).
- 161.S. J. L. Billinge, **Characterizing the structure of disordered materials**, *Symposium on "Analysis of Neutron Data of Short Range Ordered Materials" American Crystallographic Association annual meeting Buffalo* , July (1999).
- 162.S. J. L. Billinge, **Polarons in manganites; now you see them now don't**, *Workshop on the Physics of Manganites Michigan State University* , July 26-29 (1998).
- 163.S. J. L. Billinge, **Real space rietveld**, *Workshop on Local Structure from Diffraction Traverse City MI* , August 10th-14th (1997).
- 164.S. J. L. Billinge, **Studying atomic short-range order in materials: what can we learn by knowing our neighbors**, *Symposium in honor of Professor Barnett Rosenberg Michigan State University* , August 23rd (1997).
- 165.S. J. L. Billinge, **Local structure of disordered crystals from powder diffraction**, *American Crystallographic Association Annual Meeting 1997 St. Louis Missouri* , July 19-25th (1997).
- 166.S. J. L. Billinge, **Evidence of polaron formation from the local structure of  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$** , *APS March meeting Kansas City Missouri* , 17-21 March (1997).
- 167.S. J. L. Billinge, **Studying atomic short-range order in polycrystalline materials directly in real-space**, *1995 Denver X-ray Conference Denver CO* , July 31st - August 4th (1995).
- 168.S. J. L. Billinge, **Direct determination of atomic short-range order: structure-property studies of complex materials**, *Tayloring complex materials and structures CFMR spring symposium East Lansing MI* , April 9th - 10th (1995).
- 169.S. J. L. Billinge, **Probing the short-range order and dynamics of phase transitions using neutron**

**powder diffraction**, *Third Williamsburg workshop on fundamental experiments in ferroelectrics Williamsburg VA* , February 5 - 8th (1995).

- 170.S. J. L. Billinge, **Direct observation of short-range order in complex materials**, *Workshop on Defense Basic and Industrial Research at the Los Alamos Neutron Science Center Los Alamos NM* , February 12 - 15th (1995).
- 171.S. J. L. Billinge, **Local deviations from atomic long-range order and their effect on the superconductivity of high-Tc materials**, *American Crystallographic Association annual meeting Albuquerque NM* , May 23 - 28th (1993).
- 172.S. J. L. Billinge, **Local structural changes in high-Tc materials associated with superconductivity**, *Workshop on Lattice Effects in High-Tc Superconductors Santa Fe NM* , January (1992).

### *Seminars and Colloquia*

1. S. J. L. Billinge, **tbd**, *Seminar Department of Chemistry UC Davis* , Feb 9th (2016).
2. S. J. L. Billinge, **Robust prediction of real materials**, *Seminar Simons Center for Data Analysis (SCDA) Simons Foundation New York NY* , November 19th (2015).
3. S. J. L. Billinge, **The Materials Complexity Frontier: Applied Math and Computational Challenges**, *Seminar Pacific Northwest National Laboratory WA* , May 4th (2015).
4. S. J. L. Billinge, **The Materials Complexity Frontier: nanostructure and heterogeneities**, *Clearfield Endowed Lecture Texas A & M TX* , April 1st (2015).
5. S. J. L. Billinge, **The Materials Complexity Frontier: nanostructure and heterogeneities**, *Seminar Rensselaer Polytechnic Institute Albany NY* , November 21st (2014).
6. S. J. L. Billinge, **The Materials Complexity Frontier: Applied Math and Computational Challenges**, *APAM Research Conference Columbia University NY* , September 19th (2014).
7. S. J. L. Billinge, **Quantitative analysis of complex formulations with the Total Scattering Pair Distribution Function method**, *Bristo Meyers Squibb colloquium* , September 15th (2014).
8. S. J. L. Billinge, **Atomic structure at the nanoscale: from fuel cells to pharmaceuticals**, *Colloquium National Autonomous University of Mexico Mexico City Mexico* , May 7th (2014).
9. S. J. L. Billinge, **How the cat got its stripes and how hard it is to see them: search for fluctuating local C2 symmetry states in correlated oxides**, *Seminar Dept. of Physics University of Minnesota Minneapolis Minnesota* , April 30th (2014).
10. S. J. L. Billinge, **The Materials Complexity Frontier: nanostructure and heterogeneities**, *Seminar SASOL Sasolburg Orange Free State South Africa* , January 29th (2014).
11. S. J. L. Billinge, **The Materials Complexity Frontier: nanostructure and heterogeneities**, *APAM Research Conference Columbia University New York* , October 4th (2013).
12. S. J. L. Billinge, **Amorphous or nanocrystalline? Looking beyond the amorphous halo with the total scattering pair distribution function method**, *seminar Merck Rawhway NJ* , June 25th (2013).
13. S. J. L. Billinge, **PDFgui/PDFfit: Small Box modeling**, *Seminar Physics Department Queen Mary College London UK* , April 16th (2013).
14. S. J. L. Billinge, **Failed ferroelectrics: a good starting point to search for good thermoelectrics?**, *Center for Solid State Solar Thermal Energy Conversion (S3TEC) Massachusetts Institute of Technology Boston MA* , March 5th (2013).

15. S. J. L. Billinge, **Nanoscale fluctuations in bulk materials: frustrated competition and colossal responses**, *Materials Research Lecture (MRL) series lecture California Institute of Technology CA* , January 30th (2013).
16. S. J. L. Billinge, **PDF and total scattering studies: Looking at materials on the nanoscale**, *Materials Science Seminar Drexel University* , January 23rd (2013).
17. A. M. M. Abeykoon, C. D. Malliakas, P. Juhász, E. S. Bozin, M. G. Kanatzidis and S. J. L. Billinge, **The ePDF; Quantitative atomic pair distribution functions (PDFs) of nanomaterials from TEMs.**, *The 13th European Powder Diffraction Conference EPDIC Grenoble France* , 28 to 31 October The 13th European Powder Diffraction Conference (2012).
18. A. M. M. Abeykoon, C. D. Malliakas, P. Juhász, E. S. Bozin, M. G. Kanatzidis and S. J. L. Billinge, **Quantitative nanostructure characterization using atomic pair distribution functions obtained from laboratory electron microscopes**, *ICDD International Center for Diffraction Data* , 12 September (2012).
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48. S. J. L. Billinge, **Complex modeling: towards a solution of the nanostructure problem**, *SUNY-Stony Brook March 16th 2007* , (2007).
49. S. J. L. Billinge, **The nanostructure problem: what is it why do we care and what are we doing about it**, *Northwestern University March 6th 2007* , (2007).
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66. S. J. L. Billinge, **Electronic phase separation and nanoscale microstructures in correlated electron materials**, *Physics Colloquium Central Michigan University Mt. Pleasant MI* , 6th November (2003).
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