Prof. Simon J. L. Billinge
Columbia University

April 10, 2025
sb2896@columbia.edu

Education

University of Pennsylvania . . . . . Philadelphia, PA
PhD in Materials Science and Engineering . . . . . 1987 - 1992
- Advisors: Takeshi Egami and Peter Davies
- Disseration: Local atomic structure and superconducivity of $Nd_{2-x}Ce_xCuO_{4-y}$: a pair distribution function study

Oxford University . . . . . Oxford, UK
BA in Metallurgy and Materials Science . . . . . 1982 - 1986
- Disseration: Development of a novel ultra-high strength alloy steel for wire and cable

Employment

Columbia University . . . . . New York, NY
Professor . . . . . 2008 - present
- Full title: Professor of Materials Science and of Applied Physics and of Applied Mathematics

Brookhaven National Laboratory . . . . . Upton, NY
Physicist . . . . . 2008 - 2023

Institut Laue Langevin . . . . . Grenoble, France
Visiting Scientist . . . . . 2012 - 2012

European Synchrotron Radiation Facility . . . . . Grenoble, France
Visiting Scientist . . . . . 2011 - 2012

Michigan State University . . . . . East Lansing, MI
Professor . . . . . 2003 - 2007

Michigan State University . . . . . East Lansing, MI
Associate Professor . . . . . 1999 - 2003

University of Rome, 'La Sapienza' . . . . . Rome, Italy
Visiting Professor . . . . . 2001 - 2002

Michigan State University . . . . . East Lansing, MI
Assistant Professor . . . . . 1994 - 1999

Los Alamos National Laboratory . . . . . Los Alamos, NM
Director's Post-doctoral research fellow . . . . . 1992 - 1994
- Advisor: George Kwei

Awards & Honors

Gregori Aminoff prize of the Royal Swedish Academy of Sciences	2025
Innovation in Materials Characterization Award of the Materials Research Society	2025
Flack Lecturer of the Swiss Society for Crystallography	2023
Distinguished Powder Diffractionist Prize of the European Powder Diffraction Conference	2022
Warren Award of the American Crystallographic Association	2018
University of Wisconsin-Madison, School of Pharmacy, Busse Lecturer	2018
Texas A&M Clearfield Endowed Lecturer	2015
Fellow of the Neutron Scattering Society of America	2014
Neutron Scattering Society of America Service Award for outstanding service	2012
Editor of Acta Crystallographica Section A: Foundations of Crystallography	2012
Fulbright Research Scholar	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	2011
J. D. Hanawalt Award of the International Center for Diffraction Data	2010
University Distinguished Faculty Award, Michigan State University	2007
Fellow, American Physical Society	2006
Michigan State University, College of Natural Science, Distinguished Faculty Award	2006
Thomas H. Osgood Undergraduate Teaching Award	1998
Alfred P. Sloan research fellowship	1995
Sigma Xi Outstanding thesis award, U. Pennsylvania	1992
Electro-science Laboratories Award, U. Pennsylvania	1992

Major research focus area(s) and current projects.

Research Focus Areas

- Solving the nanostructure inverse problem (finding the location of atoms in nanomaterials and nanostructured bulk materials)
- Developing concepts in materials genomics, towards predictive synthesis of new materials, by developing and applying concepts in graph theory, machine learning and statistics
- Application of Machine Learning to solve otherwise intractible problems in materials characterization and discovery
- Broadening the applicability and use of the atomic pair distribution function method
- Understanding the physics of strongly correlated electron materials by studying their nanoscale electronic and magnetic textures
- Local structure property relationships of disordered crystals and nanocrystals using advanced x-ray and neutron diffraction techniques.
- Local structure of organic molecules and materials.
- More information about my research, (p)reprints, and a complete publication list, can be found at http://thebillingegroup.com/

Current Projects

AI/ML applied to solve problems in materials science . . . . . PI
Since 2015 or so, advances in AI/ML have started to have transoformational impacts on our lives in general. A question arises whether they will be useful tools to help us carry out our scientific research. In this project, we explore this question and develop AI/ML methods for carrying out better and more innovative materials science research. . . . . 2018 - present

Structure-property relationships in complex liquids and solutions . . . . . PI
Complex liquids, and liquid-liquid interactions, are at the heart of separation technologies, thermo-responsive behavior, solubility and life itself. Extracting structural information from liquids is a challenge due to the extensive averaging that takes place. This project aims to apply latest generation local structural methods and modeling, including machine learning, to gain greater insights into the complex liquid, property, relationship . . . . . 2022 - present

Education and outreach . . . . . PI
Activities in the group in education, outreach as well as diversity, equity and inclusion. . 2016 - present

A general theory of abstract system responses (gTASR) . . . . . PI
Pretty much everything is a big thing made of small things. This project explores fundamental properties that this structure imbues on a system. Because of its ubiquity (that pretty much everything has this structure) any properties that come from this general structure will need to be satisfied in a broad range of situations. This project explores the fundamental nature of systems and extends the results to a broad range of situations. . . . . 2022 - present

Local symmetry breaking in quantum materials . . . . . PI
Quantum materials are at the heart of emerging technologies from quantum computing to sustainable energy. Using local-structural methods we have developed in the group, we have found that many quantum materials exhibit local symmetry breaking: the atomic arrangements at the local scale are different to those implied by the average crystal structure. In many systems this response is intrinsic, though it can also be driven by extrinsic effects that can be controlled. This project aims to characterize these difficult to measure phenomena and, further, to understand how the local symmetry breaking affects the material properties. . . . . 2016 - present

The nanostructure inverse problem . . . . . PI
Material properties depend sensitively on the arrangements of the atoms. I.e., the atomic structure. For around 100 years we have had x-ray based tools and algorithms that allow us to solve the structure of crystalline materials: crystallography. Increasingly, we want to engineer materials at the nanoscale to give us different properties, but the nanostructure problem, the ability to solve the structure of nanomaterials, remains an unsolved problem in general. This decadal project develops experiments, algorithms, and computational methods to solve the nanostructure problem. 2016 - present

Structure of excited materials . . . . . PI
Knowledge of the structure of materials is behind our understanding of materials properties. However, the structures of materials that we solve normally are those of the material in its ground-state, i.e., its stable, relaxed state. However, in real operating devices, materials are typically not in their ground-state. In the device, a force is applied to the material which is responding to that force. To fully understand how materials are going to behave in devices, we therefore need to be able to study their structure out of the ground-state, in various excited states. These could be states where the material is responding to a voltage or physical or chemical stress. It can also be where the material is responding to a pulse of light from a laser . . . . . 2025 - present

Grants as Lead PI

Lifetime Total Grant Amount as PI: $27,778,272.63

Developing Accessible Educational and Research Resources for East African Graduate Students in Computational Materials Science and Sustainability $35,000.00
Google Research . . . . . Oct 2021 - Feb 2030

Real materials in action: Data analysis developments for real materials $900,000.00
DOE-BES . . . . . Sept 2023 - Aug 2026

A Data-driven Approach to Solving the Structure Refinement Problem for Defected and Disordered Nanoparticles $290,000.00
Toyota Research Institute . . . . . Jan 2023 - Oct 2025

Applying Machine Learning to Valuable Data in the Physical Sciences and Engineering $70,000.00
Columbia . . . . . Jul 2022 - Jun 2025

DMREF: Collaborative Research: Complex Nanofeatures in Crystals: Theory and Experiment meet in the Cloud $1,749,995.00
NSF . . . . . Oct 2019 - Sept 2024

Pair Distribution Function (PDF) Methodology and Advanced Computing for Nanostructure Determination $101,638.00
3M . . . . . Dec 2021 - Dec 2023

Conference: WORKSHOP ON SCIENTIFIC OPPORTUNITIES AND INSTRUMENTATION NEEDS FOR NEXT GENERATION MATERIALS GENOMICS BASED MATERIALS RESEARCH IN MATERIALS WITH LONG RANGE ORDER $49,153.00
NSF . . . . . Sept 2022 - Aug 2023

Towards a machine readable literature $51,500.00
International Union of Crystallography . . . . . Mar 2022 - Feb 2023

Ultrafast PDF developments $67,376.63
Brookhaven National Laboratory . . . . . Oct 2021 - Oct 2022

Development of scanning nanostructre electron microscopy $55,000.00
Johns Hopkins University . . . . . Jun 2021 - Aug 2022

X-ray Scattering $4,100,000.00
DOE-BES . . . . . Oct 2020 - Sept 2021

DMREF: Novel, data validated, nanostructure determination methods for accelerating materials discovery $1,082,785.00
NSF . . . . . Sept 2015 - Mar 2021

NOMAD as a high throughput instrument for materials genomics studies $232,514.00
ORNL . . . . . Jul 2017 - Dec 2020

X-ray Scattering $5,100,000.00
DOE-BES . . . . . Oct 2017 - Sept 2020

Nuclear Energy Enabling Technology and Nuclear Science User Facility Activities . . $70,103.00
BNL . . . . . May 2018 - Oct 2019

PDF studies of Quantum Materials $40,000.00
BNL . . . . . Oct 2017 - Sept 2018

Towards an understanding of nano-scale fluctuations in strongly correlated electron systems $2,850,000.00
DOE-BES . . . . . Oct 2014 - Sept 2017

Prediction of amorphous stability, quantification of amorphous content, and characterization of nano-particles using PDF methods $92,734.00
GlaxoSmithKline . . . . . Mar 2016 - Sept 2017

Advancing Materials Genomics: Quantifying Uncertainties for Nanostructure Determination and Optimization (QUNDO) (ROADS) $99,062.00
Columbia University . . . . . Jul 2015 - Jun 2017

Complex Modeling: leveraging data with theory and computation to push back the materials complexity frontier (Software development project) $1,500,000.00
BNL-LDRD . . . . . Jul 2012 - Jun 2015

Joint US - Africa Materials Science Institute (JUAMI) $200,000.00
NSF-DMR . . . . . Sept 2011 - Oct 2014

Towards an understanding of nano-scale fluctuations in strongly correlated electron systems $3,600,000.00
DOE-BES . . . . . Jan 2008 - Sept 2014

FRG: Beyond Crystallography: Structure of Nanostructured Materials $1,000,000.00
NSF-DMR . . . . . Aug 2007 - Jul 2011

Use of Pair Distribution Function Analysis to determine the Surface Energy of Nanoparticle Catalysts $20,228.00
Toyota Corporation and Georgia Institute of Technology . . . . . Sept 2010 - Mar 2011

Detector for new Rapid Acquisition PDF beam-line development at NSLS $279,894.00
DOE-BES . . . . . Jun 2006 - May 2009

Nanostructure determination by co-refining models to multiple data-sets $288,195.00
DOE-BES . . . . . Sept 2004 - Aug 2008

Structure of Nanocrystals $1,350,000.00
NSF-NIRT . . . . . Aug 2003 - Jul 2008

Development of medium resolution inelastic x-ray scattering (MERIX) spectrometer for the study of correlated electron systems $109,670.00
DOE-ANL . . . . . Aug 2002 - Aug 2007

Local atomic structure of functional materials using pair distribution function analysis of neutron and x-ray data $330,000.00
DOE-BES . . . . . Sept 2001 - Aug 2004

Nanoscale Inhomogenieties in Novel Electronic Materials $40,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 2003 - Jun 2004

Probing the Electronic State of Novel Materials using the Local Atomic Structure $330,000.00
NSF-DMR . . . . . Jul 2000 - Jun 2003

Local Structure-Property relationship of electronic oxides (funds a post-doc at ISIS) $200,000.00
DOE-BES . . . . . Jan 2001 - Jan 2003

Modeling molecular structure in the atomic pair distribution function $28,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 2001 - Jun 2002

Charge Inhomogeneities on Different Length-scales probed with high-resolution neutron diffraction $50,000.00
CRDF-cooperative grant program . . . . . Oct 2000 - Mar 2002

Local atomic structure of semiconductor alloys using pair distribution function analysis $431,395.00
DOE-BES . . . . . Aug 1997 - Jul 2001

Neutron Scattering Studies of Structure and Dynamics in Disordered Mesoporous Materials $155,030.00
USDC-NIST . . . . . Jul 1999 - Jun 2001

Stability and lattice dynamics of delta plutonium $26,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 2000 - Jun 2001

Cluster Refinement Method for PDF Analysis: Application to Cuprates and Manganites $20,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 2001 - Jun 2001

Local atomic structure and properties of transition metal oxides using pair distribution function analysis $270,000.00
NSF-DMR . . . . . Aug 1997 - Jul 2000

Atomic resolution of local structure in semiconductor alloys $10,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1999 - Jun 2000

A study of the local structure of transition metal oxides using pair distribution function analysis $210,000.00
lanl . . . . . Aug 1996 - Jul 1999

Modelling defects in topologically connected networks: Application to perovskite structures $13,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1998 - Jun 1999

Theoretical and Experimental studies of electronic and structural properties of pristine and doped manganites $33,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1998 - Jun 1999

Electronic and structural properties of colossal magnetoresistant oxides $66,000.00
NSF-DMR . . . . . Jan 1997 - Jan 1999

Local atomic structure of semiconductor alloys using pair distribution function analysis $13,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1997 - Jun 1998

Electronic and magnetic structure of transition metal oxides and related systems . . $45,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1997 - Jun 1998

Alfred P Sloan Research Fellowship $30,000.00
Alfred P Sloan Foundation . . . . . Dec 1995 - Dec 1997

Local atomic structure of semiconductor alloys using pair distribution function analysis $13,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1996 - Jun 1997

Electronic and magnetic structure of transition metal oxides and related systems . . $45,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1996 - Jun 1997

Local atomic structure of small clusters in host lattices $15,000.00
AURIG grant program at Michigan State University . . . . . May 1995 - Aug 1996

Local structure and properties of transition metal oxides using pair distribution function analysis $20,000.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1995 - Jun 1996

Grants as Non-Lead PI

Lifetime Subaward Grant Amount: $4,786,954.00 subaward of $65,945,639.00 total awarded.

GENESIS: A Next Generation Synthesis Center $940,000.00
DOE-BES . . . . . Aug 2018 - Jul 2024
- Role: Co-PI
- Total award: $14,850,000.00
- PI: John Parise at State University of New York, Stony Brook

Deep Generative Powder Crystallography $37,500.00
Data Science Institute @ Columbia University . . . . . Mar 2023 - Feb 2024
- Role: co-PI
- Total award: $75,000.00
- PI: Hod Lipson at Columbia University

Towards a Mechanistic Understanding of Inter- and Intra-molecular Interactions in Temperature Swing Solvent Extraction Desalination with Novel Atomistic Measurements $0.00
Columbia University . . . . . Sept 2020 - Aug 2022
- Role: Co-PI
- Total award: $42,577.00
- PI: Ngai Yin Yip at Columbia University

Unconventional Metal Organic Frameworks for actinide-lanthanide separation . . . $333,813.00
DOE-CHE . . . . . Sept 2017 - Jan 2021
- Role: Co-PI
- Total award: $333,813.00
- PI: Abraham Clearfield at Texas A&M University

Center for Precision Assembly of Superstratic and Superatomic Solids $240,000.00
NSF-DMR . . . . . Nov 2014 - Oct 2020
- Role: Co-PI
- Total award: $10,092,792.00
- PI: James Hone at Columbia University

DMREF: Collaborative Research: Designing Optimal Nanoparticle Shapes and Ligand Parameters for Polymer-Grafted Nanoparticle Membranes $300,000.00
NSF-CBET . . . . . Oct 2016 - Sept 2020
- Role: Co-PI
- Total award: $1,271,974.00
- PI: Sanat Kumar at Columbia University

Data analysis pipelines with provenance for in-situ x-ray powder diffraction and atomic pair distribution function analysis $42,577.00
BNL . . . . . Jun 2018 - May 2019
- Role: Co-PI
- Total award: $42,577.00

– PI: Line Pouchard at Brookhaven National Laboratory

Joint US-Africa Materials Advanced Studies Institute $16,769.00
NSF . . . . . Sept 2015 - Aug 2016
– Role: Co-PI
– Total award: $326,530.00
– PI: Sossina Haile at Northwestern University

PIRE:International consortium for probing novel superconductors with neutrons, muons, photons and STM $285,000.00
NSF-OISE . . . . . Aug 2010 - Jul 2015
– Role: Co-PI
– Total award: $1,820,000.00
– PI: Yasutomo Uemura at Columbia University

Re-Defining Photovoltaic Efficiency Through Molecule Scale Control $320,000.00
DOE-BES-EFRC . . . . . Oct 2009 - Aug 2014
– Role: Co-PI
– Total award: $15,254,325.00
– PI: James Hone at Columbia University

Collaborative Research: Scientific Software Innovation Institute for Advanced Analysis of X-Ray and Neutron Scattering Data (SIXNS) $100,000.00
NSF-DMR . . . . . Jul 2012 - Jun 2014
– Role: Co-PI
– Total award: $300,000.00
– PI: Brent Fultz at California Institute of Technology

Distributed Data Analysis for Neutron Scattering Experiments (Construction proposal) $1,430,000.00
NSF-IMR-MIP . . . . . Aug 2005 - Jul 2010
– Role: Co-PI
– Total award: $11,973,270.00
– PI: Brent Fultz at California Institute of Technology

Distributed Data Analysis for Neutron Scattering Experiments (Design proposal) . $121,295.00
NSF-IMR-MIP . . . . . Sept 2004 - Aug 2005
– Role: Co-PI
– Total award: $985,414.00
– PI: Brent Fultz at California Institute of Technology

Disordered oxidic and non-oxidic mesostructures $300,000.00
NSF-CHE . . . . . Aug 2002 - Jul 2005
– Role: Co-PI
– Total award: $2,232,644.00
– PI: Thomas Pinnavaia at Michigan State University

Development of the bending magnet beamlines in the MUCAT sector at the APS $0.00
DOE-BES . . . . . Sept 2000 - Aug 2003
– Role: Co-PI
– Total award: $1,200,000.00
– PI: Alan Goldman at Iowa State University

High-intensity, high-Q, high-resolution powder diffraction (H3PD) $0.00
NSF instrumentation grant . . . . . Sept 2000 - Aug 2002
– Role: Co-PI
– Total award: $800,000.00

– PI: Takeshi Egami at University of Pennsylvania

Disordered inorganic nanostructures $200,000.00
NSF-CHE . . . . . Jul 1999 - Jun 2002
– Role: Co-PI
– Total award: $1,917,858.00
– PI: Thomas Pinnavaia at Michigan State University

Disordered and lower-dimensional porous materials $120,000.00
NSF-CHE . . . . . Aug 1996 - Jul 1999
– Role: Co-PI
– Total award: $1,760,865.00
– PI: Thomas Pinnavaia at Michigan State University

Disordered and lower dimensional porous materials $0.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1997 - Jun 1998
– Role: Co-PI
– Total award: $65,000.00
– PI: Tom Pinnavaia at Michigan State University

Disordered and lower dimensional porous materials $0.00
Center for Fundamental Materials Research (CMFR) at Michigan State University Jun 1996 - Jun 1997
– Role: Co-PI
– Total award: $65,000.00
– PI: Tom Pinnavaia at Michigan State University

Wide angle capability for the high-resolution chopper spectrometer PHAROS at Los Alamos $0.00
DOE Energy Research financial assistance program . . . . . Jan 1996 - Dec 1996
– Role: Co-PI
– Total award: $536,000.00
– PI: Robert Robinson at Los Alamos National Laboratory

Graduate and Postgraduate advising

Current Ph.D. students

– Caden Myers

Graduated Ph.D. students

– Ling Lan—Graduated 2024
– Songsheng Tao—Graduated 2023
– Long Yang—Graduated 2020
– Chia-Hao (Timothy) Liu—Graduated 2020
– Soham Banerjee—Graduated 2019
– Christopher J. ”CJ” Wright—Graduated 2019
– Zizhou Gong—Graduated 2018
– Maxwell Terban—Graduated 2017
– Christopher Gutierrez—Graduated 2016
– Chenyang Shi—Graduated 2015

- Xiaohao Yang—Graduated 2015
- Timur Davis—Graduated 2011
- Ahmad Masadeh—Graduated 2008
- Hyun-Jeong Kim—Graduated 2007
- Hasan Yavas—Graduated 2007
- Moneeb Shatnawi—Graduated 2007
- Mouath Shatnawi—Graduated 2007
- He Lin—Graduated 2006
- Xiangyun Qiu—Graduated 2004
- Emil S. Bozin—Graduated 2003
- Il-Kyong Jeong—Graduated 2001
- Peter Peterson—Graduated 2001
- Remo DiFrancesco—Graduated 1999

Postdoctoral researchers and research scientists supported on grants

- Tina Na Narong- (2023 - 2025)
- Sandra H. Skjaervoe- (2020 - 2022)
- Yevgeny Rakita- (2019 - 2022)
- Robert J. Koch- (2018 - 2021)
- Ran Gu- (2017 - 2020)
- Zurab Guguchia- (2016 - 2018)
- Chung Koo Kim- (2013 - 2018)
- Runze Yu- (2016 - 2017)
- Kirsten Jensen- (2013 - 2015)
- Kevin Knox- (2011 - 2015)
- Hefei Hu- (2013 - 2014)
- Mirian García-Fernández- (2011 - 2014)
- A. M. Milinda Abeykoon- (2010 - 2013)
- Pavol Juhas- (2008 - 2012)
- Yingrui Shang- (2009 - 2011)
- Chris Farrow- (2007 - 2011)
- Emil S. Bozin- (2008 - 2010)
- Jiwu Liu- (2009 - 2010)
- Wenduo Zhou- (2006 - 2008)
- Asel Sartbaeva- (2005 - 2007)
- Gianluca Paglia- (2004 - 2006)
- Jacques Bloch- (2004 - 2005)
- Marek Schmidt- (2002 - 2004)
- Mohamed Kemali- (2000 - 2002)
- Matthias Gutmann- (1999 - 2001)
- Thomas Proffen- (1998 - 2001)
- Farida Mohiuddin-Jacobs- (1995 - 1997)

Self-funded visitors contributing to research

- Lucas Lemos Da Silva—visiting student
- Filippo Ballerini—visiting student
- Carlotta Seno—visiting student
- Till Schertenleib—visiting student
- Sara Frank—visiting student

- Martin A. Karlsen—visiting student
- Sani Harouna-Mayer—visiting student
- Emil T. S. Kjaer—visiting student
- Michael A. Waddell—adjunct scientist
- Rohan Pokratath—visiting student
- Kriti Seth—visiting student

Masters students advised

- Yucong Chen—Masters Researcher
- Sangjoon Bob Lee—Masters Researcher
- Connor Bracy—Masters Research Assistant
- Eric Shen—Masters Researcher
- Zach Thatcher—Masters Research Assistant
- Berrak Ozer—Masters Research Assistant
- Hoi Chun Chiu—Masters Researcher
- Hung T. Vuong—Masters Researcher
- Jiawei Zang—Masters Research Assistant
- Vahe Gharakhanyan—Masters Researcher
- Elizabeth Culbertson—Masters Research Assistant
- Neno Fuller—Masters Research Assistant
- Baruch Tabanpour—Masters Research Assistant
- Yarong Lin—Masters Researcher
- Hrishi Tiwari—Masters Researcher

Undergraduate research students

- Zhi Ming Xu—Undergraduate Researcher
- Samuel Andrello—Undergraduate Researcher
- John Halloram—Undergraduate Researcher
- Alison Wu—Undergraduate Researcher
- Andrew Yang—Undergraduate Research Assistant
- Rundong (Steven) Hua—Undergraduate Researcher
- Tieqiong Zhang—Undergraduate Researcher
- Zoe Zachko—Undergraduate Researcher
- David Kim Brady—Undergrad Researcher
- Adeolu Ajayi—Undergraduate Researcher
- Jaewon Lee—Undergraduate Researcher
- Evan Rowbotham—Undergraduate Researcher
- Imani Douglas—Undergraduate Research Fellow
- Eryn Dennis—Undergraduate Researcher
- Sean Wu—Undergraduate Researcher
- Kaylynn Chen—Undergraduate Researcher
- Jaylyn C. Umana—Undergraduate Research Assistant
- Robin Lee—Undergraduate Researcher
- Louis Cheng—Undergraduate Researcher
- Emily Bellingham—Undergraduate Researcher
- Adiba Ejaz—Undergraduate Research Assistant

– Priyanka Nehra—Undergraduate Researcher
– Max Zhao—Undergraduate Researcher
– Ahmed Shaaban—Undergraduate Research Assistant
– Ruby Aidun—Undergraduate Researcher
– Lauren Kranis—Undergraduate Researcher
– Daniela Hikari Yano—Undergraduate Research Assistant
– Akshay Choudhry—Undergraduate Research Assistant
– Shomik Ghose—Undergraduate Research Assistant
– Vivian Lin—Undergraduate Research Assistant
– Zicheng "Taylor" Liu—Undergraduate Research Assistant
– Michael Winitch—Undergraduate Research Assistant
– Sam Mayers—Undergraduate Research Assistant
– Nonie Thomas—Undergraduate Research Assistant
– Sasaank Bandi—Undergraduate Research Assistant
– Xin Yun—Undergraduate Research Assistant
– Xin Chen—Undergraduate Research Assistant
– Shuyue Xue—Undergraduate Research Assistant
– Justin Calamari—Undergraduate Research Assistant
– Farrah Simpson—Undergraduate Research Assistant

Service

Member of the scientific Committee of the international conference "Advances in Solid State Physics and New Materials – Celebrating 30 Years of the Center for Solid State Physics and New Materials" to be held in Belgrade, Serbia during the period May 19 to 23, 2025	2024-2025
Member of the external advisory board, of the FULL-MAP project (Furthering the development of a materials acceleration platform for sustainable batteries (combining AI, big data, autonomous synthesis robotics, high throughput testing) (Batt4EU Partnership)) at Vrije Universiteit Brussels	2024-2027
External PhD examiner for PhD student Rasmus Stubkjær Christensen of Aarhus University	2024
Review panel for Linear Coherent Light Source	2024
Review panel for National Science Foundation	2023
Co-organizer with Prof Sossina Haile (Northwestern) and Tom Mallouk (Penn State) of the fourth 2-week JUAMI Materials for Sustainable Development workshop in Nairobi, Kenya	2023
Chair and organizer for the NSF-funded workshop Scientific Opportunities and Instrumentation Needs for Next Generation Materials Genomics Based Materials Research in Materials with Long-Range Order	2022
Proposal review panel for the Department of Energy	2022
External examiner for the PhD thesis of Shuyan Zhang, co-advised by Dr. Alan McGaughey and Dr. B. Reeja Jayan in the Mechanical Engineering Department at Carnegie Mellon University	2021-2023
Office of Science (SC) Supply Chain Roundtable. Committee to study the problem of supply chain risks for scientific facilities and tools, and to suggest solutions	2021-2021
Member of the review committee of the D4 diffractometer at the Institut Laue Langevin, Grenoble, France	2021-2022

Member of the review committee Neutron Initiative of the Oak Ridge National Laboratory's Laboratory Directed Research and Development (LDRD) Program 2021-2024

External examiner for PhD thesis defense of Nasim Farahmand from the Department of Chemistry at City College 2021

Chair of the Second Target Station Instrument Review Committee of the DOE-funded Spallation Neutron Source at Oak Ridge National Laboratory. 2021

Member of the Initiative Review Committee (IRC) for the Neutron Data Interpretation Platform Ecosystem initiative at Oak Ridge National Laboratory (ORNL) 2021-2024

Member of the Future Leaders–African Independent Research (FLAIR) panel of the African Academy of Sciences panel. 2021-2023

Member of the Neutron Advisory Board (NAB) to the Neutron Sciences Directorate (NScD) or Oak Ridge National Laboratory 2021-2024

Member of the National Academy of Sciences panel reviewing the operations of the National Center for Neutron Research at NIST 2021

Member of the Hanawalt Award committee of the International Center for Diffraction Data (ICDD) 2021

Organizing committee of the meeting "Autonomous Discovery in Science and Engineering.", held at Lawrence Berkeley Laboratory. 2021

Reviewer for the Cyberinfrastructure for Sustained Scientific Innovation solicitation (CSSI) program, NSF. 2021

member of the scientific expert team for the Petra IV synchrotron development project, DESY, Hamburg, Germany. 2021-2022

Chaired the 2021 Prize Committee of the Warren Award of the American Crystallographic Association 2021

Proposal review panel for the Linear Coherent Light Source 2020

External examiner for Masters Diploma Thesis for Mr. Sani Harouna-Mayer, University of Hamburg, Germany 2020

Chair, National Science Foundation (NSF) oversight virtual site visit review team of the Center for High Energy X-ray Science (CHEXS) at the Cornell High Energy X-ray Source (CHESS) 2020

External evaluation of Anthony Phillips for promotion to Reader at Queen Mary University London 2020

Member of the International review committee of the Mantid neutron data analysis software project 2020

Co-organizer of the Chemistry, Chemical Engineering, and Materials Science track of the Machine Learning in Science & Engineering conference at Columbia University, New York, Dec 14 - 15, 2020 2020

External Thesis examiner, Nathan Nakamura, Carnegie Mellon University Department of Chemical Engineering 2020

CCQ: Machine Learning Quantum Matter Data Workshop, Flatiron Institute New York, NY 2020

Organized a symposium at the 2020 American Physical Society March Meeting entitled "Emergent local symmetry breaking in transition metal compounds due to orbital degeneracy lifting (ODL)" 2020

Review of the SNS & HFIR Data Analysis Plan 2020

Organizer, Microsymposium on Disordered materials: spectroscopic and scattering techniques at the 25th General Assembly and Congress of the International Union of Crystallography, Prague, Czech Republic, August 22-29th 2020. 2019-2020

NSF proposal review panel, SSMC CAREER Inorganics 2019

Review of the Data Reduction Handling and Analysis at the instruments suite at the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS)" at Oak Ridge National Laboratory 2019
Mentor for week-long NSF Harnessing the Data Revolution Ideas Lab workshop 2019
Organizer of a one-day JUAMI symposium on materials for sustainable energy at the 2019 African MRS meeting in Arusha, Tanzania. 2019
Member of the Italian Association of Crystallography, Commission for the Mammi Prize 2019
Italian Association of Crystallography commission for the Mammi Prize 2019
National Academy of Science Panel on the Review of the Center for Neutron Research at the National Institute of Standards and Technology 2018
Member of the External Advisory Board for NSF Science and Technology Center (STROBE) at U. Colorado 2018
Co-organizer with Prof Sossina Haile (Northwestern) and Tom Mallouk (Penn State) of the third 2-week JUAMI Materials for Sustainable Development workshop in Kampala, Uganda 2018
National Academy of Sciences Panel on the Review of the Center for Neutron Research at the National Institute of Standards and Technology 2018
Data Acquisition, Management and Analysis (DAMA) review panel, at NSLS-II, BNL 2017
Review panel for CHRNS at the NCNR at NIST 2017
Artificial intelligence task force of the Materials Research Society 2017
DISCOVER instrument advisory committee, Spallation Neutron Source, Oak Ridge National Laboratory 2017-2021
Committee to review NSF funded CHRNS program at NIST neutron reactor 2017
Data Acquisition, Management and Analysis (DAMA) group at NSLS-II 2017
Lead of the crosscutting panel on In situ characterization at the DOE-BES workshop on Basic Research Needs for Synthesis Science for Energy Relevant Technology, May 2-4, 2016 2016
Joint US/Africa Materials Initiative Materials (JUAMI) Research School, Arusha, Tanzania 2016
Powder Diffraction Beamline Review Panel, Spallation Neutron Source, Oak Ridge National Laboratory 2016
Advisory Committee, MICCoM (http://miccom-center.org/), computational materials science center Argonne National Laboratory 2016
Chair, Materials Special Interest Group of the American Crystallographic Association 2015
Steering committee of the African Light Source 2015
Symposium "Powder Pair Distribution Function and Pharmaceuticals" at ACA annual meeting, Philadelphia 2015
Triannual Review of Photon Sciences Division at Oak Ridge National Laboratory 2015
JUAMI symposium at the African-MRS, Addis Ababa, Ethiopia 2013
Chair Advanced Analysis of X-Ray and Neutron Scattering Data: Getting from data to science Workshop, Brookhaven National Laboratory 2013
Chair, microsymposium on total pattern fitting, Accuracy in Powder Diffraction Conference, NIST 2013
Chair of the J.D. Hanawalt Prize selection committee of the ICDD 2013
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

Joint US/Africa Materials Initiative Materials Research (JUAMI) School, Addis Ababa, Ethiopia	2012-2012
Chair of the NSLS-II Powder Instrument Next Generation (PING) collaboration beamline advisory team	2012-2015
Chair of the Joint US/Africa Materials Initiative Materials (JUAMI) Research School, Addis Ababa, Ethiopia	2012
Co-Chair of ZING 2012 Nanoscience Conference	2012
Chair of the symposium Amorphous, Activated and Nanomaterials at the 10th Annual Pharmaceutical Powder X-ray Diffraction Symposium (PPXRD), Lyon, France	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
Co-Chair, 2011 NSLS/CFN Joint Users' Meeting, Brookhaven National Laboratory	2011
Journal Acta Crystallographica Section A: Foundations of Crystallography	2011
International Advisory Committee, International Conference on Communication, Computational skills and Nanotechnology, Swami Ramanand Teerth Marathwada University, Nanded, Maharashtra State, India	2011
Symposium "Nanoscale Materials Diffraction" at the NSLS/CFN users meeting, Brookhaven National Laboratory	2010
Conference Chair of the American Conference on Neutron Scattering, Ottawa	2010
NSLS and NSLS-II user's executive committee	2010-2012
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
Conference Chair of the International Conference on Neutron Scattering, Knoxville, NM	2009
DOEANL Heavy Element Separation Site Review, Argonne, IL	2009
NSF-DMR review of the Center for High Resolution Neutron Scattering (CHRNS) at NIST	2009
DOE-BES review committee of Neutron scattering at Oak Ridge National Laboratory	2009
Workshop Beyond crystallography: Structure of nanostructured materials, Tempe, AZ	2008-2008
PDF beamline development team at the National Synchrotron Light Source (NSLS) beam-port X17A.	2008-2010
Chair, XPD beamline project Beamline Advisory Team (BAT), National Synchrotron Light Source II, Brookhaven National Laboratory	2008-2014
Conference Chair of the American Conference on Neutron Scattering, Santa Fe, NM	2008
Symposium, 'Under the Bonnet' Powder Diffraction Software Workshop, European Powder Diffraction Conference, Geneva, Switzerland	2006-2006
Conference chair, American Conference on Neutron Scattering, Chicago, IL	2006
Workshop participant, Cyber Infrastructure for Materials Science, NSF supported workshop to identify CI needs for the materials science community, Washington DC	2006
Member, NSF-DMR steering committee on Cyber-Infrastructure for the Materials Sciences	2005-2007
Executive Committee of the International Commission on Powder Diffraction of the Union of Crystallography	2005-2010
Neutron Scattering Society of America	2005-2010
Executive Committee of the Advanced Photon Source Users Organization	2005-2007
NSF steering committee on Cyber-Infrastructure for the materials sciences	2005-2007
ISIS facility access panel	2005-2008

Conference, “Structure of Nanocrystals”, Tempe, AZ	2004-2004
Workshop, ”Local Atomic Structure Using Neutron Pair Distribution Function (PDF) Analysis” at the American Conference on Neutron Scattering”, College Park, MD	2004-2004
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
Executive committee of the Neutron Scattering Society of America	2003-2005
Continuing Education Committee of the American Crystallographic Association	2003-2007
Symposium, “B. E. Warren Award Symposium” at the 2003 annual meeting of the American Crystallographic Association, Cincinnati	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	2003
NSLS beamtime proposal review panel	2002-2007
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	2002
Chair, Neutron scattering Special Interest Group, American Crystallographic Association	2001-2002
Workshop, Real-space Pair Distribution Function Methods, at the annual meeting of the American Crystallographic Association 2001, Los Angeles	2001-2001
Conference organizer, From Semiconductors to Proteins: beyond the average structure, Traverse City, MI.	2001
High-intensity, high-Q, high-resolution powder diffraction (H3PD) instrument for the LANSCE beamline	2000-2002
Midwest Universities Collaborative Access Team (CAT)	2000-2008
Workshop on PDF on the nanoscale, ESRF, Grenoble, France	1999-1999
Symposium, “Microstructure and Texture of Real Materials”, at the XVIIIth International Union of Crystrystallography congress and General Assembly, Glasgow, Scotland	1999-1999
Workshop, Local Structure from Diffraction, Traverse City, MI, July 1998.	1998
Conference organizer, Local Structure from Diffraction, Traverse City, MI, July 1998.	1998
Symposium Electronic Oxides: Properties and Applications, CFMR spring symposium , Michigan State University	1997
Collaboration to build a wide angle capability for the high-resolution chopper spectrometer PHAROS at Los Alamos	1996-1997

Publications

h-index:

- h = 91 (since = 1991, total citations = 36398)
  h-last five years = 54 (since = 2020, total citations = 15714)
  pulled: 4/9/2025
  Google Scholar profile
  URL:https://scholar.google.com/citations?user=dRmx8foAAAAJ&hl=en&oi=ao

1. Margalit L. Feuer, Morgan Thinel, Xiong Huang, Zhi-Hao Cui, Yinming Shao, Asish K. Kundu, Daniel G. Chica, Myung-Geun Han, Rohan Pokratath, Evan J. Telford, Jordan Cox, Emma York,

Saya Okuno, Chun-Ying Huang, Colin P. Nuckolls, Cory R. Dean, Simon J. L. Billinge, Xiaoyang Zhu, Yimei Zhu, Dmitri N. Basov, Andrew J. Millis, David R. Reichman, Abhay N. Pasupathy, Xavier Roy, and Michael E. Ziebel. "Doping Induced Charge Density Wave and Ferromagnetism in the van der Waals Semiconductor CrSBr". In: Advanced Materials (2025). arxiv.org/abs/2412.08631. URL: https://arxiv.org/abs/2412.08631.

2. Ian Henry Billinge, Gabriel D. Barbosa, Songsheng Tao, Maxwell Terban, C. Heath Turner, Simon J. L. Billinge, and Ngai Yin Yip. "A structural underpinning of the lower critical solution temperature (LCST) behavior behind temperature-switchable liquids". In: Matter 8 (2025), pp. 1–12. DOI: 10.1016/j.matt.2024.09.023. URL: https://doi.org/10.1016/j.matt.2024.09.023
3. Sara Frank, Marcel Ceccato, Henrik S. Jeppesen, Melissa J. Marks, Mads L. N. Nielsen, Ronghui Lu, Jens Jakob Gammelgaard, Jonathan Quinson, Ruchi Sharma, Julie S. Nielsen, Sara Hjelme, Cecilie Friberg Klysner, Simon J. L. Billinge, Justus Just, Frederik Gjørup, Jacopo Catalano, and Nina Lock. "The AUREX cell – a versatile operando electrochemical cell for studying catalytic materials using X-ray diffraction, total scattering, and X-ray absorption spectroscopy under working conditions". In: J. Appl. Crystallogr. (2024). submitted
4. Ling Lan, Qiang Du, and Simon J. L. Billinge. "A continuous symmetry breaking measure for finite clusters using Jensen-Shannon divergence". In: Physical Review Materials (2024). arxiv published. DOI: 10.48550/arXiv.2410.21880. URL: https://arxiv.org/abs/2410.21880
5. Till Schertenleib, Mehrdad Asgari, Beatriz Mourino, Vikram V. Karve, Timo Felder, Dragos Stoian, Volodymyr Bon, Jian Hao, Andres Ortega-Guerrero, Emad Oveisi, Kumar Varoon Agrawal, Berend Smit, Stefan Kaskel, Simon J. L. Billinge, and Wendy L. Queen. "Anisotropic node distortions in amorphous MOFs: low valent Zr sites as catalytic hotspots". In: Nature Catalysis (2024). submitted
6. Changmin Shi and Simon J. L. Billinge. "Teaching materials science and engineering students in the 21st century". In: Matter 7.12 (2024), p4130–4133. DOI: 10.1016/j.matt.2024.10.018. URL: https://doi.org/10.1016/j.matt.2024.10.018
7. Gia Thinh Tran, Allison Wustrow, Daniel O'Nolan, SongSheng Tao, Christopher J. Bartel, Tanjin He, Matthew J. McDermott, Brennan C. McBride, Karena W. Chapman, Simon J. L. Billinge, Kristin A. Persson, Gerbrand Ceder, and James R. Neilson. "Selective synthesis of defect-rich $LaMnO_3$ by low temperature anion cometathesis". In: Inorg. Chem 63.7 (2024), pp. 3250–3257. DOI: 10.1021/acs.inorgchem.3c03305. URL: https://doi.org/10.1021/acs.inorgchem.3c03305
8. Simon J. L. Billinge. "Do materials have a genome, and if they do, what can be done with it?" In: Matter 7.11 (2024), pp. 3714–3727. DOI: 10.1016/j.matt.2024.06.026. URL: https://doi.org/10.1016/j.matt.2024.06.026
9. Songsheng Tao, Jonas Billet, Jonathan De Roo, and Simon J. L. Billinge. "Rapid modeling of the local structure of metal oxide nanoparticles from PDF data: A Case Study using TiO_2 nanoparticles". In: Chem Mater (2024). DOI: 10.1021/acs.chemmater.3c03002. URL: https://pubs.acs.org/doi/full/10.1021/acs.chemmater.3c03002
10. Gabe Guo, Judah Goldfeder, Ling Lan, Aniv Ray, Albert Hanming Yang, Boyuan Chen, Simon J. L. Billinge, and Hod Lipson. "Towards end-to-end structure determination from x-ray diffraction data using deep learning". In: npj Computational Materials 10 (2024), p. 209. DOI: 10.1038/s41524-024-01401-8. URL: https://doi.org/10.1038/s41524-024-01401-8
11. Ran Gu, Yevgeny Rakita, Ling Lan, Zach Thatcher, Gabrielle E. Kamm, Daniel O'Nolan, Brennan Mcbride, Allison Wustrow, James R. Neilson, Karena W. Chapman, Qiang Du, and Simon J. L. Billinge. "Stretched non-negative matrix factorization". In: npj Comp. Mater. 10 (2024), p. 193. DOI: 10.1038/s41524-024-01377-5. URL: https://doi.org/10.1038/s41524-024-01377-5
12. Jack Griffiths, Ana Flávia Suzana, Longlong Wu, Samuel D. Marks, Vincent Esposito, Sébastien Boutet, Paul G. Evans, J. F. Mitchell, Mark P. M. Dean, David A. Keen, Ian Robinson, Simon J. L. Billinge, and Emil S. Bozin. "Resolving length-scale-dependent transient disorder

through an ultrafast phase transition". In: Nature Materials 23 (2024), pp. 1041–1047. DOI: 10.1038/s41563-024-01927-8. URL: https://doi.org/10.1038/s41563-024-01927-8
13. Gabe Guo, Tristan Luca Saidi, Maxwell W. Terban, Simon J. L. Billinge, and Hod Lipson. "Diffusion models are promising for ab initio structure solutions from nanocrystalline powder diffraction data". In: arXiv (2024). URL: https://arxiv.org/abs/2406.10796
14. Till Schertenleib, Daniel Schmuckler, Yucong Chen, Geng Bang Jin, Wendy L. Queen, and Simon J.L. Billinge. "Protocols for obtaining reliable PDFs from laboratory x-ray sources using PDFgetX3". In: arXiv (2024). DOI: 10.26434/chemrxiv-2024-9cvv0. URL: https://arxiv.org/abs/2406.18177
15. Julien Lombardi, Long Yang, Nasim Farahmand, Anthony Ruffino, Ali Younes, Jonathan E. Spanier, Simon J. L. Billinge, and Stephen O'Brien. "Structure and phase transitions in niobium and tantalum derived nanoscale transition metal perovskites, Ba(Ti,M^V)O_3, M=Nb,Ta". In: J. Chem. Phys. 160 (2024), p. 134702. DOI: 10.1063/5.0192488. URL: https://doi.org/10.1063/5.0192488
16. Simon J. L. Billinge and Thomas Proffen. "Machine learning in crystallography and structural science". In: Acta Crystallographica: Section A 80.2 (2024), pp. 102–105. DOI: 10.1107/S2053273324000172. URL: https://doi.org/10.1107/S2053273324000172
17. Emil T. S. Kjær, Andy S. Anker, Andrea Kirsch, Joakim Lajer, Olivia Aalling-Frederiksen, Simon J. L. Billinge, and Kirsten M. Ø. Jensen. "MLstructureMining: A machine learning tool for structure identification from X-ray pair distribution function data". In: Digital Discovery 3 (2024), pp. 908–918. DOI: 10.1039/D4DD00001C. URL: https://pubs.rsc.org/en/content/articlehtml/2024/dd/d4dd00001c
18. Rohan Pokratath, Kumara Cordero-Edwards, Maryame Bina, Simon Billinge, and Jonathan De Roo. "Local orthorhombic phase in zirconium oxide nanocrystals: insights from x-ray pair distribution function analysis". In: ChemRxiv (2024). DOI: 10.26434/chemrxiv-2024-9cvv0. URL: https://chemrxiv.org/engage/chemrxiv/article-details/660481aae9ebbb4db9b5dfe9
19. Simon J. L. Billinge. "JUAMI, the joint undertaking for an African materials institute: building materials science research collaborations and capabilities between continents". In: Acta Crystallographica: Section E 80.2 (2024), pp. 102–105. DOI: 10.1107/S2056989023010915. URL: https://doi.org/10.1107/S2056989023010915
20. Simon J. L. Billinge and Kirsten Jensen. Atomic pair distribution function analysis: a primer. 1st. Oxford: Oxford University Press, 2024. URL: https://global.oup.com/academic/product/atomic-pair-distribution-function-analysis-9780198885801?cc=us&lang=en&
21. Tanaporn Na Narong, Zoe N. Zachko, Steven B. Torrisi, and Simon J. L. Billinge. "Use of machine learning in experiment design for multi-modal analysis of materials: x-ray absorption near-edge spectra (XANES) and pair distribution functions (PDF)". in: arXiv (2024). arXiv:2410.17467. DOI: 10.48550/arXiv.2410.17467. URL: https://doi.org/10.48550/arXiv.2410.17467
22. Sara Frank, Mads Folkjær, Mads L. N. Nielsen, Melissa J. Marks, Henrik S. Jeppesen, Marcel Ceccato, Simon J. L. Billinge, Jacopo Catalano, and Nina Lock. "Correlating the structural transformation and properties of ZIF-67 during pyrolysis, towards electrocatalytic oxygen evolution". In: J. Maer. CHem. A 12 (2023), pp. 781–794. DOI: 10.1039/D3TA05293A. URL: https://pubs.rsc.org/en/content/articlehtml/2024/ta/d3ta05293a
23. Martin A. Karlsen, Jonas Billet, Songsheng Tao, Simon J.L. Billinge, and Dorthe B. Ravnsbæk. "Operando pair distribution function analysis of nanocrystalline functional materials: the case of TiO2-bronze nanocrystals in Li-ion battery electrodes". In: J. Appl. Crystallogr. (2023)
24. Emil T. S. Kjær, Andy S. Anker, Marcus N. Weng, Simon J. L. Billinge, Raghavendra Selvan, and Kirsten M. Ø. Jensen. "DeepStruc: Towards structure solution from pair distribution function data using deep generative models". In: Digital Discovery 2 (2023), pp. 69–80. DOI: 10.1039/D2DD00086E. URL: https://doi.org/10.1039/D2DD00086E
25. Andy S. Anker, Ulrik Friis-Jensen, Frederik L. Johansen, Simon J. L. Billinge, and Kirsten

M. Ø. Jensen. “ClusterFinder: A fast tool to find cluster structures from pair distribution function data”. In: Acta Crystallogr. A 80.2 (2023), pp. 213–220. DOI: 10.1107/S2053273324001116. URL: https://doi.org/10.1107/S2053273324001116

26. Ian K. Robinson, Jack P. Griffiths, Robert Koch, Tadesse A. Assefa, Ana F. Suzana, Yue Cao, Sungwon Kim, Dongjin Kim, Heemin Lee, Sunam Kim, Jae Hyuk Lee, Sang-Youn Park, Intae Eom, Jaeku Park, Daewoong Nam, Sangsoo Kim, Sae Hwan Chun, Hyojung Hyun, Kyung sook Kim, Ming Lu, Changyong Song, Hyunjung Kim, Simon J. L. Billinge, and Emil S. Bozin. “Emergence of liquid following laser melting of gold thin films”. In: IUCrJ 12.6 (2023), pp. 656–661. DOI: 10.1107/S2052252523009363. URL: https://doi.org/10.1107/S2052252523009363
27. Mitra L. Taheri, Elaf Anber, Annie Barnett, Simon J. L. Billinge, Nick Birbilis, Brian DeCost, Daniel L. Foley, Emily Holcome, Jonathan Hollenbach, Howie Joress, Georgia Leigh, Yevgeny Rakita, James M. Rondinelli, Nathan Smith, Michael J. Waters, and Chris Wolverton. “Understanding and leveraging short-range order in compositionally complex alloys”. In: MRS Bulletin 48 (2023), pp. 1280–1291. DOI: 10.1557/s43577-023-00591-8. URL: https://doi.org/10.1557/s43577-023-00591-8
28. Anton Kovyakh, Soham Banerjee, Chia-Hao Liu, Christopher J. Wright, Yuguang C. Li, Thomas E. Mallouk, Robert Feidenhans’l, and Simon J. L. Billinge. “Towards scanning nanostructure x-ray microscopy”. In: J. Appl. Crystallogr. 56 (2023), pp. 1221–1228. DOI: 10.1107/S1600576723005927. URL: https://doi.org/10.1107/S1600576723005927
29. E. S. Bozin, H. Xie, A. M. M. Abeykoon, S. M. Everett, M. G. Tucker, M. G. Kanatzidis, and S. J. L. Billinge. “Local Sn Dipolar-Character Displacements behind the Low Thermal Conductivity in SnSe Thermoelectric”. In: Phys. Rev. Lett. 131 (2023), p. 036101. DOI: 10.1103/PhysRevLett.131.036101. URL: https://doi.org/10.1103/PhysRevLett.131.036101
30. Ana F. Suzana, Robert Koch, Longlong Wu, Tadesse A. Assefa, Sungwon Kim, Sungwook Choi, Heemin Lee, Sunam Kim, Jae Hyuk Lee, Sang-Youn Park, Daewoong Nam, Sangsoo Kim, Hyojung Hyun, Kyung Sook Kim, Gwen Wright, Emil S. Bozin, Changyong Song, Hyunjung Kim, Simon J. L. Billinge, and Ian K. Robinson. “Compressive effects in melting of Palladium thin films studied by ultrafast x-ray diffraction”. In: Phys. Rev. B 107 (2023), p. 214303. DOI: 10.1103/PhysRevB.107.214303. URL: https://journals.aps.org/prb/abstract/10.1103/PhysRevB.107.214303
31. Rohan Pokratath, Laurent Lermusiaux, Stefano Checchia, Jikson Pulparayil Mathew, Susan Rudd Cooper, Jette Katja Mathiesen, Guillaume Landaburu, Soham Banerjee, Songsheng Tao, Nico Reichholf, Simon J. L. Billinge, Benjamin Abécassis, Kirsten M. Ø. Jensen, and Jonathan De Roo. “An amorphous phase precedes crystallization: unraveling the colloidal synthesis of zirconium oxide nanocrystals”. In: ACS Nano 17.9 (2023), pp. 8796–8806. DOI: 10.1021/acsnano.3c02149. URL: https://doi.org/10.1021/acsnano.3c02149
32. Ran Gu, Simon J. L. Billinge, and Qiang Du. “A fast two-stage algorithm for non-negative matrix factorization in smoothly varying data”. In: Acta Crystallogr.: Section A 79.2 (2023), pp. 203–216. DOI: 10.1107/S2053273323000761. URL: https://onlinelibrary.wiley.com/iucr/doi/10.1107/S2053273323000761
33. Simon A. J. Kimber, Jiayong Zhang, Charles H. Liang, Gian G. Guzmán-Verri, Peter B. Littlewood, Yongqiang Cheng, Douglas L. Abernathy, Jessica M. Hudspeth, Zhong-Zhen Luo, Mercouri G. Kanatzidis, Tapan Chatterji, Anibal J. Ramirez-Cuesta, and Simon J. L. Billinge. “Dynamic crystallography reveals spontaneous anisotropy in cubic GeTe”. In: Nature Materials 22 (2023), 311–315 (2023). DOI: 10.1038/s41563-023-01483-7. URL: https://www.nature.com/articles/s41563-023-01483-7
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37. Andy S. Anker, Emil T. S. Kjær, Mikkel Juelsholt, Troels Lindahl Christiansen, Susanne Linn Skjærvø, Mads Ry Vogel Jørgensen, Innokenty Kantor, Daniel Risskov Sørensen, Simon J. L. Billinge, Raghavendra Selvan, and Kirsten M. Ø. Jensen. "Extracting structural motifs from pair distribution function data of nanostructures using explainable machine learning". In: npj Computational Materials 8 (2022), p. 213. DOI: 10.1038/s41524-022-00896-3. URL: https://doi.org/10.1038/s41524-022-00896-3
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39. Sani Y. Harouna-Mayer, Songsheng Tao, ZiZhou Gong, Ann-Christin Dippel, Martin von Zimmermann, Dorota Koziej, and Simon J. L. Billinge. "Real space texture and pole figure analysis using the three-dimensional pair distribution function on a platinum thin film". In: IUCrJ 9.5 (2022), pp. 594–603. DOI: 10.1107/S2052252522006674. URL: https://doi.org/10.1107/S2052252522006674
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Presentations

1. Simon J. L. Billinge, Frontiers of local structure determination and prospects for ai to extend them, First Latin American Powder Diffraction Conference (LAPDiC), Fortaleza, Brazil, October 11–14$^{\text{th}}$ (2025).
2. Simon J. L. Billinge, AI/ML in crystallography: what can it do for us, what can we do with it?, 35th Europan Crystallographic Meeting, Posnan, Poland, August 25–29$^{\text{th}}$ (2025).
3. Simon J. L. Billinge, AI at your service: ai tools for solving crystallographic problems, Transactions Symposium at the 75th American Crystallographic Association Annual Meeting, Lombard, Illinois, July 18–23$^{\text{rd}}$ (2025).
4. Simon J. L. Billinge, Real materials in action: studying structure on different length and time-scales, 10th European Crystallography School, ESC10, Ohrid, North Macedonia, June 22–27$^{\text{th}}$ (2025).
5. Simon J. L. Billinge, Tracking local order and dynamics in functional materials, Advances in Solid State Physics and New Materials Symposium, Institute of Physics, Serbian Academy of Sciences, Belgrade, Serbia, May 17–24$^{\text{th}}$ (2025).
6. Simon J. L. Billinge, Watching real materials in action: everything, everywhere, all at once, Materials Research Society Spring Meeting Prize Symposium, Seattle, WA, April 9$^{\text{th}}$ (2025).
7. Simon J. L. Billinge, Local structure on the move: emerging methods to study local dynamics, Seminar, Department of Materials Science, University of California Santa Barbara, Santa Barbara CA, March 6$^{\text{th}}$ (2025).
8. Simon J. L. Billinge, Watching real materials in action: everything, everywhere, all at once, Gregori Aminoff prize presentation 2025, Lund, Sweden, March 2$^{\text{nd}}$ (2025).
9. Simon J. L. Billinge, Watching real materials in action: everything, everywhere, all at once, Bruker-AXS / MIT Symposium 2025: Non-Bragg Methods for Your In-House Source, Massachusetts Institute of Technology, Boston, MA, February 21–22$^{\text{nd}}$ (2025).
10. Simon J. L. Billinge, Atomic pair distribution function tutorial, Bruker-AXS / MIT Symposium

2025: Non-Bragg Methods for Your In-House Source, Massachusetts Institute of Technology, Boston, MA, February 21–22nd (2025).

11. Simon J. L. Billinge, Studying real materials in action: time resolved measurements of local structure in materials at synchrotrons and xfels, The African Synchrotron Light Source (AfLS7-2024) Conference, Johannesburg, South Africa, (Webinar), November 18–21st (2024).
12. Simon J. L. Billinge, All density functional theory (DFT) is wrong, Sagamore XX - 2024, Shiv Nadar Institution of Eminence - Delhi NCR, India, November 10–17th (2024).
13. Simon J. L. Billinge, Real materials in action: studying structure on different length and time-scales, Japanese national institute for materials science (NIMS) annual award symposium, Tsukuba, Japan, November 5–8th (2024).
14. Simon J. L. Billinge, Watching real materials in action: everything, everywhere, all at once, Colloquium, Materials Department, University of California Santa Barbara, Santa Barbara CA, October 7–8th (2024).
15. Simon J. L. Billinge, Real materials in action: everything, everywhere, all at once, Colloquium, Department of Physics, Rensselaer Polytechnic Institute, Troy NY, September 18th (2024).
16. Simon J. L. Billinge, Materials genomics, materials heredity and the structure definition problem, MACSMIN 2024, University of Liverpool, UK, (Webinar), September 9–13th (2024).
17. Simon J. L. Billinge, AI in material structure research: basics and applications, Swedish-German Røntgen-Ångstrom cluster (RÅC) conference on "X-ray and neutron research on bio-inspired materials and sustainable energy technology, Krakow, Poland, September 1–8th (2024).
18. Simon J. L. Billinge, AI at your service, Eighteenth European Powder Diffraction Conference (EPDIC18) 2024, Padova, Italy, August 30–2nd (2024).
19. Simon J. L. Billinge, Big box, small box, black box, George Box, 34th European Crystallographic Meeting (ECM34), Padova, Italy, August 26–30th (2024).
20. Simon J. L. Billinge, Updates on pdf modeling software with diffpy-cm, Software Fayre of the European Powder Diffraction Conference (EPDIC) 18, Padova, Italy, August 26–30th (2024).
21. Simon J. L. Billinge, Intrinsic quantum textures: broken local symmetry in quantum materials, MGI-PI meeting, Washington DC, July 30–31st (2024).
22. Simon J. L. Billinge, Do materials have a genome, and if they do, what can be done with it?, Joint USA-European Symposium on Machine learning, simulations and experiments for ultra low-power materials and devices, Spetses Island in Greece, July 14–19th (2024).
23. Simon J. L. Billinge, Ai and machine learning for powder crystallographers, International School of Crystallography "Powder diffraction: Real materials in the information era, Erice, Italy, May 31–7th (2024).
24. Simon J. L. Billinge, Powder diffraction beyond powders, International School of Crystallography "Powder diffraction: Real materials in the information era", Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Italy, May 31–7th (2024).
25. Simon J. L. Billinge, The materials genome and the search for universal and continuous structure representations, SIAM Conference on Mathematical Aspects of Materials Science (MS24), Pittsburg, PA, May 19–23rd (2024).
26. Simon J. L. Billinge, Supervised and unsupervised machine learning applied to challenging and rapid diffraction and structural problems, Symposium Machine Learning Methods, Data and Automation for Sustainability and Electronics at the Spring meeting of the Materials Research Society, Seattle, WA, April 22–26th (2024).
27. Simon J. L. Billinge, Seeing structuring in liquids using advances in atomic pair distribution function methods, Award symposium in honor of Jarad Mason at the Spring 2024 American Chemical Society Meeting, New Orleans, LA, March 17–21st (2024).
28. Simon J. L. Billinge, Real materials in action: data analysis developments for real materials doing real things, 2024 Neutron Scattering Principal DOE Investigators' Meeting, Rockville, MD, January 10–12th (2024).

29. Simon J. L. Billinge, Intrinsic quantum textures: quantifying local symmetry breaking from the atomic pair distribution function analysis of x-ray and neutron diffraction data, Disorder and Quantum Phases of Matter Workshop, Aspen Center for Physics, Aspen, CO, December 11–15$^{\text{th}}$ (2023).
30. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts via saving the planet: understanding nanostructure with x-rays and algorithms, Colloquium, Department of Physics, Indiana University, Bloomington IN, December 6$^{\text{th}}$ (2023).
31. Simon J. L. Billinge, Prospects for autonomous materials discovery guided by in situ diffraction, Emerging Challenges and Opportunities in Materials by Design Symposium, Fall meeting of the Materials Research Society, Boston, MA, November 26–1$^{\text{st}}$ (2023).
32. Simon J. L. Billinge, Watching real materials in real devices with the atomic pair distribution function (PDF), The African Synchrotron Light Source (AfLS6-2023) Conference, Johannesburg, South Africa, (Webinar), November 13–17$^{\text{th}}$ (2023).
33. Simon J. L. Billinge, Watching real materials in real devices with the atomic pair distribution function (PDF),, Howard Flack Award Lecture, Dectris, Baden, Switzerland, November 10$^{\text{th}}$ (2023).
34. Simon J. L. Billinge, Local structural analysis when a material has spatial, temporal and orientational heterogeneities, Howard Flack Award Lecture, Paul Scherrer Institute, Switzerland, November 10$^{\text{th}}$ (2023).
35. Simon J. L. Billinge, Real materials in action: studying structure on different length and timescales, Howard Flack Award Lecture, ETH, Zurich, Switzerland, November 9$^{\text{th}}$ (2023).
36. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts via saving the planet: understanding nanostructure with x-rays and algorithms, Howard Flack Award Lecture, University of Basel, Basel, Switzerland, November 8$^{\text{th}}$ (2023).
37. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts via saving the planet: understanding nanostructure with x-rays and algorithms, Howard Flack Award Lecture, University of Bern, Bern, Switzerland, November 7$^{\text{th}}$ (2023).
38. Simon J. L. Billinge, Real materials in action: studying structure on different length and timescales, Howard Flack Award Lecture, EPFL Sion, Switzerland, November 6$^{\text{th}}$ (2023).
39. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts: understanding nanostructure with x-rays and algorithms, Seminar, Materials Science, California Institute of Technology, Pasadena CA, October 17–18$^{\text{th}}$ (2023).
40. Simon J. L. Billinge, Handling heterogeneity in materials structure characterization: approaches to separate signals using multiple spaces, APAM department research conference, Columbia University, September 22$^{\text{nd}}$ (2023).
41. Simon J. L. Billinge, Handling heterogeneity: approaches to separate signals using multiple spaces, Advanced Data Analysis Methodologies workshop at the 2023 Annual Meeting of the Societa Italiana Luce di Sincrotroni (SILS), Universita di Roma "La Sapienza", Rome, Italy, August 30–1$^{\text{st}}$ (2023).
42. Simon J. L. Billinge, The atomic pair distribution (PDF) method: application to pharmaceuticals, Seminar, Excelsus-Novartis bimonthly seminars at St Johann Campus, Excelsus Structural Solutions (Swiss) AG, Basel None, August 24–25$^{\text{th}}$ (2023).
43. Simon J. L. Billinge, Tips and tricks for better coding of figures in python using matplotlib, 2023 IUCr Crystallographic Computing School, Melbourne, Australia, (Webinar), August 19–22$^{\text{nd}}$ (2023).
44. Simon J. L. Billinge, AI and machine learning aided extraction of static and dynamic local structural information from total scattering data, Data-Driven Design of Energy Materials Workshop at the American Chemical Society (ACS) Fall Meeting, San Francisco, August 13–17$^{\text{th}}$ (2023).
45. Simon J. L. Billinge, Total scattering: materials beyond crystallography, Croucher Summer Course on Neutron Scattering, City University of Hong Kong, Kowloon, Hong Kong, August 8–12$^{\text{th}}$ (2023).
46. Simon J. L. Billinge, Neutron diffraction and structure refinement, Croucher Summer Course on

Neutron Scattering (CSC), City University of Hong Kong, Hong Kong, August 6–12th (2023).

47. Simon J. L. Billinge, Introduction to materials characterization, JUAMI School on Materials Science for Sustainable Energy Applications, University of Nairobi, Nairobi, Kenya, June 19–30th (2023).
48. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts via saving the planet: understanding nanostructure with x-rays and algorithms, Seminar, Department of Chemistry, University of Sheffield, Sheffield None, May 25–26th (2023).
49. Simon J. L. Billinge, Do materials have a genome, and if they do, what can we do with it?, MACSMIN (Mathematics and Computer Science for Materials Innovation), University of Liverpool, Liverpool, UK, May 22–26th (2023).
50. Simon J. L. Billinge, Characterizing amorphous and nanostuctured materials with total scattering, 3rd Spring Pharmaceutical Synchrotron-XRPD workshop (SPS-XRPD-3), Purdue University, (Webinar), May 19–20th (2023).
51. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts via saving the planet: understanding nanostructure with x-rays and algorithms, Seminar, School of Chemistry, University of Birmingham, Birmingham None, May 18th (2023).
52. Simon J. L. Billinge, Ultrafast atomic pair distribution function analysis, Time-resolved X-ray Opportunities toward APS-U, Argonne National Laboratory, (Webinar), May 3–4th (2023).
53. Simon J. L. Billinge, Autonomation for scientific discovery: beamline experiments of the future, what they might look like and how to get there, Toward Synchrotron-Based Autonomous Scattering Studies of Synthesis and Processing workshop at the Advanced Photon Source (APS)/Center for Nanoscale Materials (CNM) annual User Meeting, Argonne National Laboratory, Argonne, IL, (Webinar), May 1–2nd (2023).
54. Simon J. L. Billinge, When hard materials act soft: local symmetry breaking in materials, how to find it, and why you should care about it, Colloquium, Condensed Matter Physics Department, Paul Scherrer Institute, Villigen None, (Webinar), April 28th (2023).
55. Simon J. L. Billinge, AI and machine learning aided prompt analysis of powder diffraction and PDF data, Real-time Analysis of Synchrotron Light Source and Nanoscale Research Center Data using AI/ML for APS-U First Experiments workshop at the 2023 APS/CNM Users Meeting, Argonne National Laboratory, Argonne, IL, (Webinar), April 19–20th (2023).
56. Simon J. L. Billinge, Treasure from trash: algorithms to help hard x-rays handle hard experimental situations, Seminar, Photon Sciences Division Seminar, Brookhaven National Laboratory, Upton NY, (Webinar), April 18th (2023).
57. Simon J. L. Billinge, AI and machine learning aided prompt analysis of powder diffraction and PDF data, Machine Learning for X-ray and Neutron Scattering Workshop on April 17th and 18th, Lawrence Berkeley National Laboratory, Berkeley CA, April 17–18th (2023).
58. Simon J. L. Billinge, Local structural analysis when a material has spatial, temporal and orientational heterogeneities, Seminar, ISIS spallation neutron source, Rutherford Appleton Laboratory, Harwell Oxfordshire, March 29th (2023).
59. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts via saving the planet: understanding nanostructure with x-rays and algorithms, Colloquium, Department of Chemistry, Weizmann Institute, Tel Aviv None, March 13–15th (2023).
60. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts via saving the planet: understanding nanostructure with x-rays and algorithms, Seminar, Istituto di cristallografia, Consiglio Nazionale delle Ricerche, Bari None, February 7th (2023).
61. Simon J. L. Billinge, Ultrafast atomic pair distribution function analysis, Scientific opportunities with very hard XFEL radiation, DESY, Hamburg, Germany, January 18–20th (2023).
62. Simon J. L. Billinge, Ultra fast atomic pair distribution function (PDF) analysis: a new chapter in the goal of atomic movies, AfLS Conference, Johannesburg, South Africa, (Webinar), November 14–18th (2022).
63. Simon J. L. Billinge, Pavol Juhas, Songsheng Tao, Diffpy-cmi - a software toolbox for real-space

structure analysis , School and conference on analysis of diffraction data in real space, Grenoble, France, October 16–22nd (2022).

64. Simon J. L. Billinge, Recent and future developments in PDF-land, School and conference on analysis of diffraction data in real space, Grenoble, France, October 16–22nd (2022).
65. Simon J. L. Billinge, Progress in PDF for structural characterization of nanomaterials, Workshop on electron PDF (ePDF), Center for Research in Energy and Materials (CNPEM), Campinas, Brazil, (Webinar), October 10–11th (2022).
66. Simon J. L. Billinge, Do materials have a genome, and if they do, what can we do with it?, Lectures in Quantum Crystallography and Related Fields, IUCR Quantum Crystallography Commission, (Webinar), September 29th (2022).
67. Simon J. L. Billinge, Community coding practices for scientific software: tips and tricks for making better code and having it outlive your participation in the project, Computational methods in the Structural Sciences workshop, 2022 SSRL/LCLS Users meeting, (Webinar), September 26–30th (2022).
68. Simon J. L. Billinge, Unsupervised and supervised machine learning for total scattering and PDF analyses, , Columbia University, (Webinar), September 23rd (2022).
69. Simon J. L. Billinge, Using synchrotrons to study structure-property relationships in complex nanostructured materials, LAAAMP-AfLS Africa Workshop, ujohannesburg, (Webinar), September 8th (2022).
70. Simon J. L. Billinge, Unsupervised and supervised machine learning for total scattering and pdf analyses, 33rd European Crystallographic Meeting (ECM33), symposium Computations with/for Pair Distribution Functions, Versailles, Paris, France, August 23–27th (2022).
71. Simon J. L. Billinge, azunger, Qiang Du, xroy, Intrinsic local symmetry breaking in materials: implications for MGI, NSF DMREF PI meeting 2022, College Park, MD, June 27–28th (2022).
72. Simon J. L. Billinge, Total scattering and atomic pair distribution function analysis: overview and applications, International School of Crystallography, Diffuse scattering: the crystallography of dynamics, defects, and disorder, Erice, Italy, June 3–11th (2022).
73. Simon J. L. Billinge, The nanostructure inverse problem in the time of artificial intelligence, The Distinguished Powder Diffractionist award presentation of the European Powder Diffraction Conference (EPDIC), Šibenik, Croatia, May 31–3rd (2022).
74. Simon J. L. Billinge, Characterizing structure in sticky situations: atomic pair distribution function (PDF) analysis , Seminar, 3M Technical Forum seminar, 3M, St. Paul MN, (Webinar), May 24th (2022).
75. Simon J. L. Billinge, From saving pharmaceuticals to saving priceless historical artefacts via saving the planet: understanding nanostructure with x-rays and algorithms, Seminar, Department of Chemistry, University of Milan, Milan None, May 20th (2022).
76. Simon J. L. Billinge, When hard materials act soft: local symmetry breaking in bulk materials, how to find it, and why you should care about it, Seminar, Department of Science and Advanced Technology, Università degli Studi dell'Insubria, Como None, May 11th (2022).
77. Simon J. L. Billinge, X-ray characterization of amorphous, nanocrystalline and heterogeneous products using atomic pair distribution function (PDF) analysis, Rigaku Pharma Forum, Rigaku Headquarters, Neu-Isenburg, Frankfurt, Germany, (Webinar), April 27–28th (2022).
78. Simon J. L. Billinge, Characterizing amorphous and nanostuctured materials with total scattering pair distribution function analysis, Rigaku Pair Distribution Function Workshop, Online, (Webinar), April 6–7th (2022).
79. Ling Lan, Sandra H. Skjaervoe, Simon J. L. Billinge, Classification and determination of octahedral tilts in perovskites using a machine learning approach, Columbia University Data Science Day 2022, New York, NY, April 6th (2022).
80. Simon J. L. Billinge, Keeping up with the data: accelerating materials discovery in a high data velocity world, Seminar, Department of Materials Science and Engineering, Boston University,

Boston MA, (Webinar), December 10th (2021).

81. Simon J. L. Billinge, Recent and upcoming developments in PDF analysis, 2nd US School on Total Scattering Analysis, Oak Ridge National Laboratory, (Webinar), October 25–29th (2021).
82. Chia-Hao (Timothy) Liu, Christopher J. "CJ" Wright, Zach Thatcher, Songsheng Tao, Yevgeny Rakita, phuck, donolan, mbeauvais, svornholt, okononova, rmcauliffe, gveith, pchupas, gceder, kpersson, kchapman, Simon J. L. Billinge, Next generation tools to interrogate, predict & control synthesis, DOE-BES EFRC PI meeting, Gaithersburg, MD, (Webinar), October 18–19th (2021).
83. Simon J. L. Billinge, Mapping nanostructure at the micro and nanoscale with the help of x-rays and applied math, Seminar, APAM Research Conference, Columbia University, New York NY, October 15th (2021).
84. Emil T. S. Kjaer, aanker, Simon J. L. Billinge, rselvan, Kirsten Jensen, Automated characterization of the atomic structure of mono-metallic nanoparticles from x-ray scattering data using generative models, DANSCATT meeting, Lyngby, Denmark, October 8–9th (2021).
85. Simon J. L. Billinge, Structural studies with total scattering, Danscatt Users Meeting, The Technical University of Denmark, Copenhagen, Denmark, (Webinar), October 8–9th (2021).
86. Simon J. L. Billinge, Introduction to PDF analysis and applications of PDF analysis, ToscaLand total scattering workshop, Granada, Spain, (Webinar), September 20–24th (2021).
87. Simon J. L. Billinge, PDFgui hands on demonstration, ToscaLand total scattering workshop, Grenada, Spain, (Webinar), September 20–24th (2021).
88. Emil T. S. Kjaer, aanker, Simon J. L. Billinge, rselvan, Kirsten Jensen, Automated characterization of the atomic structure of mono-metallic nanoparticles from x-ray scattering data using generative models, phd seminar, copenhagen, denmark, September 10th (2021).
89. Simon J. L. Billinge, Application of non negative matrix factorization NMF, Crystallographic Computing School of the IUCr, Prague, Czech Republic, (Webinar), September 1–3rd (2021).
90. Simon J. L. Billinge, Songsheng Tao, Advanced modeling of nanostructure from atomic pair distribution functions (PDFs) using diffpyCMI, Crystallographic Computing School of the IUCr, Prague, Czech Republic, (Webinar), September 1–3rd (2021).
91. Simon J. L. Billinge, Contributing to community codes: GitHub workflow for community software development, Crystallographic Computing School of the IUCr, Prague, Czech Republic, (Webinar), September 1–3rd (2021).
92. Simon J. L. Billinge, Zach Thatcher, Packaging and distributing your code, Crystallographic Computing School of the IUCr, Prague, Czech Republic, (Webinar), September 1–3rd (2021).
93. Simon J. L. Billinge, Testing your code: test driven development, Crystallographic Computing School of the IUCr, Prague, Czech Republic, (Webinar), September 1–3rd (2021).
94. Simon J. L. Billinge, Keeping up with the data: accelerating discovery in a high data velocity world with the help of machine learning, Workshop on Data Science and Machine Learning in Chemistry, University of Copenhagen, Copenhagen, Denmark, August 30–3rd (2021).
95. Lucas B. M. Pinheiro, Elizabeth Culbertson, Gabriel L. B. de Araujo, Simon J. L. Billinge, Fabio Furlan Ferreira, Effect of grinding procedures on the ritonavir-lopinavir system, IUCr quadrennial Congress, Prague, Czech Republic, (Webinar), August 14–22nd (2021).
96. Martin A. Karlsen, Simon J. L. Billinge, PDFitc, structureMining and similarityMapping demo, IUCr25, Software Fayre, Prague, Czech Republic, August 14–22nd (2021).
97. Martin A. Karlsen, Berrak Ozer, Simon J. L. Billinge, pyDataRecognition demo, IUCr25, Software Fayre, Prague, Czech Republic, August 14–22nd (2021).
98. Simon J. L. Billinge, Moving towards a more data-centric scientific literature: pilot with IUCr, pydatarecognition , IUCr quadrennial Congress Software Fayre, Prague, Czech Republic, (Webinar), August 14–22nd (2021).
99. Simon J. L. Billinge, Atomic pair distribution function (PDF) in the cloud, IUCr quadrennial Congress Software Fayre, Prague, Czech Republic, (Webinar), August 14–20th (2021).
100. Simon J. L. Billinge, Advanced modeling of nanostructure from atomic pair distribution functions

(PDFs) using diffpyCMI on windows 10, IUCr quadrennial Congress Software Fayre, Prague, Czech Republic, (Webinar), August 14–20th (2021).

101. Yevgeny Rakita, James L. Hart, Partha Das, Stavros Nicolopoulos, Mitra Taheri, Simon J. L. Billinge, Scanning nano-structure electron microscopy - hidden potential for evolving systems, IUCr quadrennial Congress, Prague, Czech Republic, (Webinar), August 14–22nd (2021).
102. Simon J. L. Billinge, Keeping up with the data: accelerating discovery in a high data velocity world, Joint Nanoscience and Neutron Science User Meeting, Oak Ridge National Laboratory, (Webinar), August 10th (2021).
103. Emil T. S. Kjaer, aanker, Simon J. L. Billinge, rselvan, Kirsten Jensen, Automated characterization of the atomic structure of mono-metallic nanoparticles from x-ray scattering data using generative models, DTU, DIKU & AAU summer school on geometric deep learning, Vejle, denmark, July 16–20th (2021).
104. Simon J. L. Billinge, Local structure from diffraction with the help of epithermal neutrons, Canadian Institute for Neutron Scattering's virtual seminar series, Canada, June 24th (2021).
105. Emil T. S. Kjaer, aanker, andrea kirsch, Simon J. L. Billinge, Kirsten Jensen, Automated phase characterization for pair distribution function data, Smart Lighthouse workshop on atomic structure of functional materials, Sandbjerg, Denmark, June 14–17th (2021).
106. Simon J. L. Billinge, When hard materials act soft: local symmetry breaking in quantum materials, how to find it, and why you should care about it, Quantum Materials: New Insights from Neutron Scattering, University of Minnesota Center for Quantum Materials, (Webinar), June 9–10th (2021).
107. Simon J. L. Billinge, Challenges for US-Africa international collaboration involving computing, JUAMI-Open Computing Facility Symposium Panel on Equitable Access to Computing, UC Berkeley, (Webinar), May 19–20th (2021).
108. Simon J. L. Billinge, Keeping up with the data: accelerating discovery in a high data velocity world, Machine Learning Augmented X-Ray Scattering and Spectroscopies Workshop at the 2021 NSLS-II & CFN Users' Meeting, Brookhaven National Laboratory, May 17–20th (2021).
109. Simon J. L. Billinge, Towards the autonomation of experiments: quasi-real time analysis of heterogeneous streaming data from scientific experiments, Virtual Research Day 2021, Initiative for Computational Science and Engineering (iCSE), Columbia University, New York, NY, (Webinar), May 12th (2021).
110. Simon J. L. Billinge, Advanced data analytics in the service of structure science, convolutional neural networks for space-group classification and beyond, Seminar, Materials Science and Engineering Department, Technion-Israel Institute of Technology, Haifa None, (Webinar), April 29th (2021).
111. Simon J. L. Billinge, Reflections on the DANSE software project, Neutron Scattering Society Neutron Cafe, California Institute of Technology, Pasadena, CA, (Webinar), April 1st (2021).
112. Simon J. L. Billinge, Local symmetry breaking in crystals: nature, origins and consequences, Atomic-level characterization of hybrid perovskites (HPATOM), University of Cambridge, Cambridge, UK, (Webinar), January 26–28th (2021).
113. Emil T. S. Kjaer, aanker, Kirsten Jensen, rselvan, Simon J. L. Billinge, Characterising the atomic structure of mono-metallic nanoparticles from x-ray scattering data using conditional generative models, Machine Learning in Science & Engineering 2020, New York, NY, (Webinar), December 14–15th (2020).
114. Chia-Hao (Timothy) Liu, Yunzhe Tao, Hung T. Vuong, Daniel Hsu, Qiang Du, Simon J. L. Billinge, Using a machine learning approach to determine the space group of a structure from the atomic pair distribution function, Machine Learning in Science and Engineering Conference, Columbia University, December 14–15th (2020).
115. Simon J. L. Billinge, PDF perspectives from the past to the future, PDF-2020, a two-day celebration of the pair distribution function for scientific research, Shanghai, China, (Webinar), December 4–5th (2020).

116. Simon J. L. Billinge, irobinson, Dynamics and control in complex oxides: towards ultra-fast pair distribution analysis (ufPDF) studies, DOE BES x-ray scattering PI meeting, Online, (Webinar), November 9–11$^{\text{th}}$ (2020).
117. Simon J. L. Billinge, Emil S. Bozin, irobinson, Hidden broken symmetries: local structure and domains, DOE BES x-ray scattering PI meeting, Online, (Webinar), November 9–11$^{\text{th}}$ (2020).
118. Simon J. L. Billinge, Opportunities for diffraction-based temporally and spatially resolved nanostructure studies in situ with small beams, Petra IV workshop Structure of Nanomaterials and Nanoparticles during Growth, In-situ and Operando Conditions, DESY, Hamburg, (Webinar), November 4$^{\text{th}}$ (2020).
119. Simon J. L. Billinge, Prospects for scattering (towards Moire), Beyond Epitaxy: New Moire platforms, Army Research Office online virtual workshop, (Webinar), October 30$^{\text{th}}$ (2020).
120. Simon J. L. Billinge, Orbital degeneracy lifting: broken local symmetries and their orderings in interesting electronic materials, Colloquium, Materials Research Laboratory, California Institute of Technology, Pasadena CA, (Webinar), October 28$^{\text{th}}$ (2020).
121. Simon J. L. Billinge, Local and nanoscale structure from AI and computationally enhanced pair distribution function (PDF) diffraction data, Seminar, Department of Physics, Universidade Federal do ABC, Santo André None, (Webinar), September 29$^{\text{th}}$ (2020).
122. Emil T. S. Kjaer, aanker, Kirsten Jensen, rselvan, Simon J. L. Billinge, Characterising the atomic structure of mono-metallic nanoparticles from x-ray scattering data using conditional generative models, Artificial Intelligence in Chemistry, Virtual, (Webinar), August 28–29$^{\text{th}}$ (2020).
123. Emil T. S. Kjaer, aanker, Kirsten Jensen, rselvan, Simon J. L. Billinge, Characterising the atomic structure of mono-metallic nanoparticles from x-ray scattering data using conditional generative models, KDD International Workshop on Mining and Learning with Graphs, Virtual, (Webinar), August 24$^{\text{th}}$ (2020).
124. Simon J. L. Billinge, Solving the climate crisis one PDF at a time, Seminar, Center for Computational Mathematics, The Flatiron Institute, New York NY, (Webinar), July 16$^{\text{th}}$ (2020).
125. Simon J. L. Billinge, Scanning nanostructure electron microscopy (SNEM), USA Webinar Series, NanoMEGAS, (Webinar), June 16$^{\text{th}}$ (2020).
126. Simon J. L. Billinge, Machine learning material symmetry, and recipes from precious data, Columbia DSI - Flatiron Institute research opportunities workshop, Flatiron Institute, 162 Fifth Avenue, New York, NY, March 3$^{\text{rd}}$ (2020).
127. Simon J. L. Billinge, On the origins, ubiquity and the need for a new language to classify correlated disorder, Correlated Disorder Workshop, Paul Scherrer Institute, Herzberg, Switzerland, February 24–27$^{\text{th}}$ (2020).
128. Simon J. L. Billinge, Efficient capture of metadata during experiments. why, when and how?, National Synchrotron Light Source II Friday lunchtime seminar series, Brookhaven National Laboratory, Upton, NY, February 14$^{\text{th}}$ (2020).
129. Simon J. L. Billinge, Machine learning material symmetry, and recipes from precious data, Seminar, Data Science Institute, Columbia University, New York NY, February 13$^{\text{th}}$ (2020).
130. Simon J. L. Billinge, Machine learning materials science from experimental and theoretical data, Workshop on Machine Learning Quantum Matter Data, Center for Computational Quantum Physics (CCQ) of the Flatiron Institute, New York, NY, January 23–24$^{\text{th}}$ (2020).
131. Simon J. L. Billinge, Clusters, cluster-mining, and teaching machines to study nanostructure, Seminar, Department of Physics and Astronomy, Michigan State University, East Lansing MI, January 18–21$^{\text{st}}$ (2020).
132. Simon J. L. Billinge, Characterizing structure when your material is disordered or nanostructured: yes you can, African Materials Research Society Meeting, Arusha, Tanzania, December 10–13$^{\text{th}}$ (2019).
133. Simon J. L. Billinge, Towards clusterography, a crystallography for our 21st century materials, Colloquium, Department of Chemistry and Chemical Biology, Harvard University, Cambridge MA,

October 24th (2019).

134. Simon J. L. Billinge, Clusters, cluster-mining, and cluster assembly structures from advanced x-ray scattering measurements, Seminar, Center for Precision Assembly of Superstratic and Superatomic Solids (PAS3), Columbia University, New York NY, October 1st (2019).
135. Simon J. L. Billinge, Local structure of real materials, Seminar, Department of Applied Physics and Applied Mathematics, Columbia University, New York NY, September 20th (2019).
136. Simon J. L. Billinge, Atomic pair distribution function (PDF) analysis of nanostructured and disordered materials, Chemistry of Materials Lectureship & Best Paper Award symposium, American Chemical Society Fall Meeting, San Diego, CA, August 25–29th (2019).
137. Simon J. L. Billinge, Towards a human and machine-readable scientific literature, Workshop on Data Science Skills in Publishing: for authors, editors and referees, Vienna, Austria, August 18th (2019).
138. Simon J. L. Billinge, Atomic and magnetic pair distribution function methods, Workshop on Advanced Powder Diffraction, Uppsala, Sweden, August 12–Aug14th (2019).
139. Simon J. L. Billinge, Hands-on PDF and mPDF tutorials, Workshop on Advanced Powder Diffraction, Uppsala, Sweden, August 12–Aug14th (2019).
140. Simon J. L. Billinge, Orbital degeneracy lifting, broken local symmetries and their orderings, Workshop on Competing Interactions and Colossal Responses in Transition Metal Oxides and Related Compounds, Telluride, CO, June 24–29th (2019).
141. Simon J. L. Billinge, Computed tomography PDF (ctPDF): digging up buried nanostructures, Neutron Scattering Gordon Research Conference, Hong Kong, May 5–10th (2019).
142. Simon J. L. Billinge, Think local, act global: when hard materials act soft, Workshop on low-energy structural and electronic dynamics in soft semiconducting materials, Tel Aviv, Israel, May 2nd (2019).
143. Simon J. L. Billinge, When hard materials act soft: local symmetry breaking in materials, how to find it, and why you should care about it, Colloquium, Physics, Brigham Young University, Provo UT, April 13th (2019).
144. Simon J. L. Billinge, Recent and future developments in PDF-land, School and conference on analysis of diffraction data in real space, Grenoble, France, March 17–23rd (2019).
145. Simon J. L. Billinge, When hard materials act soft: local symmetry breaking in materials, how to find it, and why you should care about it, Colloquium, Department of Physics, Kent State University, Kent OH, March 14th (2019).
146. Simon J. L. Billinge, Atomic pair distribution function (PDF) analysis of nanostructured and disordered materials, Seminar, Department of Chemistry, Rice University, Houston TX, February 18th (2019).
147. Simon J. L. Billinge, Synchrotron x-rays: helping build communities and get drugs to market, 2nd Pan African Conference on Crystallography and the 2nd African Light Source Project Workshop, Accra, Ghana, January 28–22nd (2019).
148. Christopher J. "CJ" Wright, Line Pouchard, Simon J. L. Billinge, Reproducibility for streaming analysis, The International Conference for High Performance Computing, Networking, Storage, and Analysis, Dallas, TX, November 11–16th (2018).
149. Simon J. L. Billinge, Robust prediction of real material structure, Colloquium, Department of Physics and Astronomy, University of Delaware, Newark DE, October 31st (2018).
150. Simon J. L. Billinge, Fluctuating valence bonds in strongly interacting systems: hard to find but then hard to ignore, Seminar, Department of Physics, Columbia University, New York NY, October 19th (2018).
151. Simon J. L. Billinge, Materials discovery is more than materials prediction: the role of light-sources in addressing the materials synthesis data gap, Gap Analysis: Materials Discovery through Data Science at Advanced User Light Sources, Santa Fe, NM, October 3–5th (2018).
152. Simon J. L. Billinge, Total scattering and atomic pair distribution function analysis: overview and

applications, Hot topics in contemporary crystallography - HTCC2018, Bol, Croatia, September 23–27th (2018).

153. Simon J. L. Billinge, Total scattering and atomic pair distribution function analysis: overview and applications, NSLS-II Pair Distribution Function School 2018, Brookhaven National Laboratory, Upton, NY 11973, September 17–Sep19th (2018).
154. Simon J. L. Billinge, Building PDF refinement scripts using diffpy-cmi code, European Crystallographic Computing Forum 2018, Mieres, Spain, August 18–22nd (2018).
155. Simon J. L. Billinge, On collaborative tools and repositories, European Crystallographic Computing Forum 2018, Mieres, Spain, August 18–22nd (2018).
156. Simon J. L. Billinge, Software development workflow for robust software, European Crystallographic Computing Forum 2018, Mieres, Spain, August 18–22nd (2018).
157. Simon J. L. Billinge, Emil S. Bozin, Local and intermediate range symmetry breaking, who cares? the properties!, Effects in Multiferroics Beyond the Coupling of Magnetic and Electric Order, 2018 Gordon Conference on Multiferroic and Magnetoelectric Materials, Bates College, Lewiston, ME, August 5–10th (2018).
158. Simon J. L. Billinge, A series of fortunate events: how the pdf method went from niche technique to mainstream and beyond, Research Experience for Undergraduates Seminar Series, Columbia University, New York, NY, July 26th (2018).
159. Simon J. L. Billinge, pduxbury, Some theoretical and computational aspects of nanocluster structure solution, American Crystallographic Association Annual meeting, Toronto, Ontario, Canada, July 20–25th (2018).
160. Simon J. L. Billinge, A series of fortunate events: how the PDF method went from niche technique to mainstream and beyond, American Crystallographic Association Annual meeting, Toronto, Ontario, Canada, July 20–25th (2018).
161. Soham Banerjee, Simon J. L. Billinge, Atomic pair distribution function (PDF) analysis of nanostructured and disordered materials, 5th Annual NYU X-ray Workshop, New York, NY, June 27th (2018).
162. Simon J. L. Billinge, A series of fortunate events: how the atomic pair distribution function method went from niche technique to mainstream and beyond, and how this was unlocked by synchrotron radiation, UKSR50: 50 years of Synchrotron Radiation in the UK and its global impact, University of Liverpool, Liverpool, UK, June 26–29th (2018).
163. Christopher J. "CJ" Wright, Simon J. L. Billinge, Pavol Juhas, lpouchard, Provenance-enabled sample measurements and tracking for multi-modal analysis and predictive synthesis., 2018 NSLS-II and CFN Users Meeting, Upton, NY, May 22–24th (2018).
164. Elizabeth Culbertson, Simon J. L. Billinge, Total scattering characterization of organic materials using the pair distribution function, 2018 NSLS-II and CFN Users Meeting, Upton, NY, May 22–24th (2018).
165. Soham Banerjee, tliu, Simon J. L. Billinge, ClusterMining: determining metallic nanoparticle core structures from atomic pair distribution function data, 2018 NSLS-II and CFN Users Meeting, Upton, NY, May 22–24th (2018).
166. Simon J. L. Billinge, Recent developments in PDF analysis of organics and pharmaceuticals, Pharmaceutical studies with data gathered from synchrotron x-ray powder diffraction, Purdue University, West Lafayette, IN, May 8–9th (2018).
167. Simon J. L. Billinge, Finding and controlling atoms at the nanoscale for better drug delivery, Busse Lecture of the School of Pharmacy, University of Wisconsin, Madison, WI, May 2–5th (2018).
168. Simon J. L. Billinge, Amorphous or nanocrystalline? advances in the total scattering pair distribution function methods for characterizing amorphous and nanocrystalline pharmaceuticals,, Colloquium, Department of Pharmaceutical Sciences, University of Wisconsin-Madison, Madison WI, May 2–5th (2018).
169. Simon J. L. Billinge, PDF then, now and in the pipeline, University of Copenhagen Total

Scattering Symposium, University of Copenhagen, Copenhagen, Denmark', April 23–29th (2018).

170. Simon J. L. Billinge, Opportunities for nanostructure determination with the PDF method, Columbia MRSEC IRG2 meeting, Columbia University, March 29th (2018).
171. Elizabeth Culbertson, Simon J. L. Billinge, Atomic pair distribution function (PDF) analysis of Co-Se superatoms, Columbia MRSEC IRG2 meeting, Columbia University, March 29th (2018).
172. Christopher J. "CJ" Wright, Simon J. L. Billinge, Algorithms and approaches for robust PDFs, Mini Workshop on ePDF, Ulm University, Ulm, Germany, March 24–29th (2018).
173. Simon J. L. Billinge, On the robustness of atomic pair distribution function (PDF) models, 26th Annual Meeting of the German Crystallographic Society (DGK), Essen, Germany, March 4–9th (2018).
174. Simon J. L. Billinge, Recent developments from PDFland: new methods for nanostructure determination, Seminar, Institute for Solid State Physics, Max Planck Institute, Stuttgart None, March 4–9th (2018).
175. Simon J. L. Billinge, Juami: the joint understanding for an african materials institute, African Materials Research Society Meeting, Gaberone, Botswana, December 5–12th (2017).
176. Simon J. L. Billinge, Synchrotron x-rays: helping build communities and get drugs to market, Science Forum South Africa, Pretoria, South Africa, December 5–12th (2017).
177. Simon J. L. Billinge, tbd, Data Science Institute retreat, Tarrytown, NY, October 1–2nd (2017).
178. Christopher J. "CJ" Wright, Simon J. L. Billinge, An introduction to ePDF experiments, analysis, and modeling., Seminar, Biology, Chemistry & Earth Sciences, Universität Bayreuth, Bayreuth None, March 26th (2017).

Memberships

American Physical society . . . . . Mar 1990-present
Fellow

American Crystallographic Association . . . . . Jun 1991-present
Member

Materials Research Society . . . . . Aug 1991-present
Member

Neutron Scattering Society of America . . . . . May 1993-present
Fellow

Association for Computing Machinery . . . . . Mar 2015-present
Member

American Chemical Society . . . . . Mar 2023-present
Member