

Simon J. L. Billinge

Professional Preparation.

University of Oxford	Oxford, UK	Materials Science	BA	1986
University of Pennsylvania	Philadelphia, PA	Materials Science and Eng.	PhD	1992
Los Alamos Natl. Laboratory	Los Alamos, NM	Solid State Physics	Post-doc	1992-94

Appointments.

2008-present	Professor of Materials Science and Applied Physics and Applied Mathematics, Columbia University
2008-present	Scientist, Brookhaven National Laboratory
2003-2007	Professor of Physics, Michigan State University
2001-2002	Visiting Professor, University of Rome, 'La Sapienza'
1999-2003	Associate Professor of Physics, Michigan State University
1994-1999	Assistant Professor of Physics, Michigan State University
1992-1994	Director's Post-doctoral Research Fellow, Los Alamos National Laboratory

Societies

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

Current Research Interests

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

Products.

TEN REPRESENTATIVE PUBLICATIONS

1. T. Egami and S. J. L. Billinge, *Underneath the Bragg peaks: structural analysis of complex materials*, 2nd Ed., Elsevier, Amsterdam, 2012. (total citations for both editions >1000)
2. C. L. Farrow, P. Juhás, Jiwu Liu, D. Bryndin, E. S. Bozin, J. Bloch, Th. Proffen and S. J. L. Billinge, **PDFfit2 and PDFgui: Computer programs for studying nanostructure in crystals**, *J. Phys: Condens. Mat.* **19**, 335219 (2007). (citations > 750, total citations for all software > 2000)
3. S. J. L. Billinge and I. Levin, **The problem with determining atomic structure at the nanoscale**, *Science* **316**, 561-565 (2007). doi: 10.1126/science.1135080 (citations ~ 400)
4. E. S. Bozin, C. D. Malliakas, P. Souvatzis, T. Proffen, N. A. Spaldin, M. G. Kanatzidis and S. J. L. Billinge, **Entropically stabilized local dipole formation in lead chalcogenides**, *Science* **330**, 1660 (2010). doi: 10.1126/science.1192759 (citations ~150)
5. Joshua J. Choi, Xiaohao Yang, Zachariah M. Norman, Simon J. L. Billinge and Jonathan S. Owen, **Structure of methylammonium lead iodide on mesoporous titanium dioxide: active material in high performance metal-organic solar cells**, *Nano Lett.* **14**, 127-133 (2014). (citations >150 since 2014).
6. Jianwei Miao, Peter Ercius and Simon J. L. Billinge, **Atomic electron tomography: 3D structures without crystals**, *Science* **353**, aaf2157 (2016)
7. P. Juhás, D. M. Cherba, P. M. Duxbury, W. F. Punch and S. J. L. Billinge, **Ab initio determination of solid-state nanostructure**, *Nature* **440**, 655-658 (2006). doi: 10.1038/nature04556
8. Alexander N. Beecher, Octavi E. Semonin, Jonathan M. Skelton, Jarvist M. Frost, Maxwell W. Terban, Haowei Zhai, Ahmet Alatas, Jonathan S. Owen, Aron Walsh and Simon J. L. Billinge, **Direct**

- observation of dynamic symmetry breaking above room temperature in methylammonium lead iodide perovskite**, *ACS Energy Lett.* **1**, 880–887 (2016).
9. Kirsten M. O. Jensen, Pavol Juhás, Marcus A. Tofanelli, Christine L. Heinecke, Gavin Vaughan, Christopher J. Ackerson and Simon J. L. Billinge, **Polymorphism in magic sized $\text{Au}_{144}(\text{SR})_{60}$ clusters**, *Nat. Commun.* **7**, 11859 (2016).
 10. Michael Ghidui, Michael Naguib, Chenyang Shi, Olha Mashtalir, Limei Pan, Bo Zhang, Jian Yang, Yury Gogotsi, Simon J. L. Billinge and Michel W. Barsoum, **Synthesis and characterization of two-dimensional Nb_4C_3 (MXene)**, *Chem. Commun.* **50**, 9517-9520 (2014).

Synergistic activities:

1. Non-traditional classroom teaching- Since 2012 I have been teaching my classes at Columbia using a flipped classroom and employing peer instruction methods. Students are expected to read background material and watch videotaped lectures before class. Classroom time is then spent discussing concepts. This has led to improvements in outcomes as measured by better performance on exams (a definite shift upwards of the central portion of the grade distribution curve compared to similar exams taught previously using the old lecture style). The students also like the class, giving good instructor grades for enjoyment as well as quantity learned.
2. Community education and training- We run regular hands-on workshops to train people to use PDF methods and programs. We also host workshops and extended student and colleague visits to MSU to learn these techniques. For example, a workshop is planned for the summer of 2017, organized in collaboration with Oak Ridge National Laboratory.
3. Community Scientific Software Efforts - We developed and maintain the widely used Diffpy (www.diffpy.org) suite of Programs for atomic pair distribution function analysis of materials. This includes the highly successful PDFgui program and the powerful and actively developed CMI (Complex Modeling Infrastructure) program as well as a number of data reduction and analysis programs. We are also developing software for data collection and analysis at the XPD diffractometer at NSLS-II synchrotron at Brookhaven National Laboratory. All the public codes are hosted at GitHub in the DIFFPY and xpdAcq collaborations, respectively.
4. Recent review Panels and Community Service Powder Diffraction Beamline Review Panel, Spallation Neutron Source, Oak Ridge National Laboratory, August (2016), Panel Lead, DOE-BES Basic Research Needs Workshop, Rockville MD, May (2016), Advisory Committee, MICCoM (<http://miccom-center.org/>), computational materials science center Argonne National Laboratory (2016-), Triannual Review of Photon Sciences Division at SNS (2015).
5. Undergrad research in the group – We now target the involvement of undergrads in research in the lab, working under the direct mentorship of grad students and overseen by myself. In particular, we have targeted women and minorities. In the past two years we have mentored the following students: Ophira Blumna (Barnard), Emily J Bellingham, Farrah Simpson, Shuyue Xue, Derek Tropf, Justin Calamari, Xian Yang (all Columbia, 2016-17), Joseph Kaming-Thanassi (high school, summer 2016), Caleb Duff (BYU, summer 2016), Daniel Puttnam, Carlos Martin, Derek Tropf, Justin Calamari, Adam Jaffe, Xian Yang, Erica Yee (all Columbia, 2015-16), Sarah Stone (Brooklyn Institute of Technology 2015), which includes six women. I am also mentoring an African American student, Neno Fuller as part of the Columbia University Bridge to PhD program.