Prof. Simon J. L. Billinge
Columbia University

March 13, 2021
sb2896@columbia.edu

Publication Listing

1. Mengtan Liu, Ryan D. McGillicuddy, Hung Vuong, Songsheng Tao, Adam H. Slavney, Miguel I. Gonzalez, **Simon J. L. Billinge**, and Jarad A. Mason. "Network-Forming Liquids from Metal–Bis(acetamide) Frameworks with Low Melting Temperatures". In: *J. Amer. Chem. Soc.* (2021). to be published. DOI: 10.1021/jacs.0c11718. URL: https://doi.org/10.1021/jacs.0c11718

2. Henrik L. Andersen, Benjamin A. Frandsen, Haraldur P. Gunnlaugsson, Mads R. V. Jørgensen, **Simon J. L. Billinge**, Kirsten M. Ø. Jensen, and Mogens Christensen. "Local and long-range atomic/magnetic structure of non-stoichiometric spinel iron oxide nanocrystallites". In: *IUCrJ* 8.1 (2021), pp. 2052–2525. DOI: 10.1107/S2052252520013585. URL: https://doi.org/10.1107/S2052252520013585

3. A. Altomare and **S. J. L. Billinge**. "Modern crystallography and its foundations". In: *Acta Crystallogr. A* 77.1 (2021), p. 1. DOI: 10.1107/S2053273320016678. URL: https://doi.org/10.1107/S2053273320016678

4. Ran Gu, Qiang Du, and **Simon J. L. Billinge**. "A fast two-stage algorithm for non-negative matrix factorization in streaming data". In: *IEEE Trans. Signal Process.* (2021). arXiv:2101.08431 [math.OC]. URL: https://arxiv.org/abs/2101.08431

5. Jeremy L. Hitt, Yuguang C. Li, Songsheng Tao, Zhifei Yan, Yue Gao, **Simon J. L. Billinge**, and Thomas E. Mallouk. "A High Throughput Optical Method for Studying Composition Effects in Electrochemical CO_2 Reduction Catalysts". In: *Nature Commun.* (2021). to be published

6. Christopher "CJ" Wright, Songsheng Tao, and **Simon J. L. Billinge**. "SHED: Streaming Heterogeneous Event Data Tracking with Provenance". In: *J. Open Source Software* (2021). submitted. DOI: 10.21105/joss.02796. URL: https://github.com/openjournals/joss-papers/blob/joss.02796/joss.02796/10.21105.joss.02796.pdf

7. Long Yang, Elizabeth A. Culbertson, Nancy K. Thomas, Hung T. Vuong, Emil T. S. Kjær, Kirsten M. Ø. Jensen, Matthew G. Tucker, and **Simon J. L. Billinge**. "A cloud platform for atomic pair distribution function analysis: PDFitc". In: *Acta Crystallogr. A* 77.1 (2021), pp. 2–6. DOI: 10.1107/S2053273320013066. URL: https://journals.iucr.org/a/issues/2021/01/00/ae5091/index.html

8. Jingjing Yang, Jake Russell, Songsheng Tao, Martina Lessio, Feifan Wang, Alaina Hartnett, Samuel Peurifoy, Evan Doud, Evan O'Brien, Natalia Gadjieva, David Reichman, X-Y. Zhu, Andrew Crowther, **Simon Billinge**, Xavier Roy, Michael Steigerwald, and Colin Nuckolls. "Superatomic Solid Solutions". In: *Nature Chem.* (2021). to be published

9. Zhi Wang, Xin-Gang Zhao, Robert Koch, **Simon J. L. Billinge**, and Alex Zunger. "Understanding electronic peculiarities in tetragonal FeSe as local structural symmetry breaking". In: *Phys. Rev. B* 102.23 (2020), p. 235121. DOI: 10.1103/PhysRevB.102.235121. URL: https://link.aps.org/doi/10.1103/PhysRevB.102.235121

10. Long Yang, Robert J. Koch, Hong Zheng, John F. Mitchell, Weiguo Yin, Matthew G. Tucker, **Simon J. L. Billinge**, and Emil S. Bozin. "Two-orbital degeneracy lifted local precursor to a

metal-insulator transition in $MgTi_2O_4$". In: *Phys. Rev. B* 102.23 (2020), p. 235128. DOI: 10.1103/PhysRevB.102.235128. URL: https://journals.aps.org/prb/abstract/10.1103/PhysRevB.102.235128

11. Chia-Hao Liu, Eric Janke, Li Ruipen, Pavol Juhás, Oleg Gang, Dimitri V. Talapin, and **Billinge, Simon J. L.** "sasPDF: pair distribution function analysis of nanoparticle assemblies from small-angle-scattering data". In: *J. Appl. Crystallogr.* (2020). arXiv:1910.08186 [cond-mat.mtrl-sci]. URL: https://arxiv.org/abs/1910.08186

12. Yevgeny Rakita, Daniel O'Nolan, Rebecca McAuliffe, Gabriel Veith, Peter Chupas, **Billinge, Simon**, and Karena Chapman. "Active Reaction Control of Cu Redox State Based on Real-Time Feedback from *in situ* Synchrotron Measurements". In: *J. Am. Chem. Soc.* 142.44 (2020), 18758–18762. DOI: 10.1021/jacs.0c09418. URL: https://pubs.acs.org/doi/10.1021/jacs.0c09418

13. Paul K. Todd, Allison Wustrow, Rebecca D. McAuliffe, Matthew J. McDermott, Gia Thinh Tran, Brennan C. McBride, Ethan D. Boeding, Daniel O'Nolan, Chia-Hao Liu, Shyam S. Dwaraknath, Karena W. Chapman, **Simon J. L. Billinge**, Kristin A. Persson, Ashfia Huq, Gabriel M. Veith, and James R. Neilson. "Defect-accommodating intermediates yield selective low-temperature synthesis of $YMnO_3$ polymorphs". In: *Inorg. Chem.* 59 (2020), 13639–13650. DOI: 10.1021/acs.inorgchem.0c02023. URL: https://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.0c02023

14. Daniel O'Nolan, Guanglong Huang, Gabrielle E. Kamm, Antonin Grenier, Chia-Hao Liu, Paul Todd, Allison Wustrow, Gia Thinh Tran, David Montiel, James R. Neilson, **Simon J. L. Billinge**, Peter J. Chupas, Katsuyo S. Thornton, and Karena W. Chapman. "A thermal-gradient approach to variable-temperature measurements resolved in space". In: *J. Appl. Crystallogr.* 81 (2020), pp. 39–55. DOI: 10.1107/S160057672000415X. URL: http://scripts.iucr.org/cgi-bin/paper?S160057672000415X

15. Long Yang, Pavol Juhás, Maxwell W. Terban, Matthew G. Tucker, and **Billinge, Simon J. L.** "Structure-mining: screening structure models by automated fitting to the atomic pair distribution function over large numbers of models". In: *Acta Crystallogr. A* 76.3 (2020), pp. 395–409. DOI: 10.1107/S2053273320002028. URL: https://journals.iucr.org/a/issues/2020/03/00/vk5039/

16. Maxwell Terban, Luca Russo, Tran Pham, Dewey Barich, Yan Sun, Matthew Burke, Jeffrey Brum, and **Billinge, Simon**. "Local structural effects due to micronization and amorphization on an HIV treatment active pharmaceutical ingredient". In: *Molecular Pharmaceutics* 17.7 (2020), pp. 2370–2389. DOI: 10.1021/acs.molpharmaceut.0c00122. URL: https://doi.org/10.1021/acs.molpharmaceut.0c00122

17. Line Pouchard, Pavol Juhas, Gilchan Park, Huub Van Dam, Stuart I. Campbell, Eli Stavitski, **Simon Billinge**, and Christopher J. Wright. "Provenance infrastructure for multi-modal x-ray experiments and reproducible analysis". In: *Handbook on Big Data and Machine Learning in the Physical Sciences*. Singapore: World Scientific, 2020, pp. 307–331. DOI: 10.1142/9789811204579_0015. URL: https://doi.org/10.1142/9789811204579_0015

18. Andy S. Anker, Emil T. S. Kjaer, Eric B. Dam, **Simon J. L. Billinge**, Kirsten M. Ø. Jensen, and Raghavendra Selvan. "Characterising the atomic structure of mono-metallic nanoparticles from x-ray scattering data using conditional generative models". In: *KDD* (2020). Accepted to the conference International Workshop on Deep Learning on Graphs (KDD-DLG). Available on ChemArxiv (doi is 10.26434/chemrxiv.12662222). DOI: 10.26434/chemrxiv.12662222. URL:

https://chemrxiv.org/articles/preprint/Characterising_the_Atomic_Structure_of_Mono-Metallic_Nanoparticles_from_X-Ray_Scattering_Data_Using_Conditional_Generative_Models/12662222/1

19. Tadesse A. Assefa, Yue Cao, Soham Banerjee, Sungwon Kim, Dongjin Kim, Heemin Lee, Sunam Kim, Jae Hyuk Lee, Sang-Youn Park, Intae Eom, Jaeku Park, Daewoog Nam, Sangsoo Kim, Sae Hwan Chun, Hyojung Hyun, Kyung Sook Kim, Pavol Juhas, Emil S. Bozin, Ming Lu, Changyong Song, Hyunjung Kim, **Simon J. L. Billinge**, and Ian K. Robinson. "Melt-front Dynamics in Polycrystalline Gold Thin Films". In: *Science Adv.* 6.3 (2020), eaax2445. DOI: 10.1126/sciadv.aax2445. URL: https://advances.sciencemag.org/content/6/3/eaax2445/tab-pdf

20. Soham Banerjee, Chia-Hao Liu, Kirsten M. O. Jensen, Pavol Juhás, Jennifer D. Lee, Christopher J. Ackerson, Christopher B. Murray, and **Billinge, Simon J. L.** "Cluster-mining: An approach for determining core structures of metallic nanoparticles from atomic pair distribution function data". In: *Acta Crystallogr. A* 76.1 (2020), pp. 24–31. DOI: 10.1107/S2053273319013214. URL: https://doi.org/10.1107/S2053273319013214

21. Yue Cao, Tadesse Assefa, Soham Banerjee, Andrew Wieteska, Dennis Wang, Abhay Pasupathy, Xiao Tong, Yu Liu, Wenjian Lu, Yu-Ping Sun, Yan He, Xiaojing Huang, Hanfei Yan, Yong S. Chu, **Simon J. L. Billinge**, and Ian K. Robinson. "Complete Strain Mapping of Nanosheets of Transition Metal Chalcogenides". In: *ACS Appl. Mater. Interf.* (2020). to be published. DOI: 10.1021/acsami.0c06517. URL: https://doi.org/10.1021/acsami.0c06517

22. R. J. Koch, R. Sinclair, M. T. McDonnell, R. Yu, M. Abeykoon, M. G. Tucker, A. M. Tsvelik, **S. J. L. Billinge**, H. D. Zhou, W.-G. Yin, and E. S. Bozin. "Dual Orbital Degeneracy Lifting in a Strongly Correlated Electron System". In: *arXiv* (2020). 2009.14288 [cond-mat.str-el]

23. Chia-Hao Liu, Christopher J. Wright, Ran Gu, Sasaank Bandi, Allison Wustrow, Paul K. Todd, Daniel O'Nolan, Michelle L. Beauvais, James R. Neilson, Peter J. Chupas, Karena W. Chapman, and **Simon J. L. Billinge**. "Validation of non-negative matrix factorization for rapid assessment of large sets of atomic pair-distribution function (PDF) data". In: *J. Appl. Crystallogr.* (2020). arXiv:2010.11807 [cond-mat.mtrl-sci]. URL: https://arxiv.org/abs/2010.11807

24. **Simon J. L. Billinge**. "21st century crystallography challenges: structure beyond crystals". In: *IUCr newsletter*. Ed. by Michael Glazer. Vol. 27. 4. 2019, p. 7. URL: https://www.iucr.org/news/newsletter/etc/articles?issue=145052&result_138339_result_page=7

25. Robert E. Dinnebier and **Billinge, Simon J. L.** "Overview and principles of powder diffraction". In: *International Tables of Crystallography*. Ed. by Christopher Gilmore, James Kaduk, and Henk Schenk. Vol. H. Chester, UK: International Union of Crystallography, 2019. Chap. 1.1, pp. 2–23. DOI: 10.1107/97809553602060000935. URL: https://it.iucr.org/Ha/ch1o1v0001/

26. Sheng-Han Lo, Liang Feng, Kui Tan, Zhehao Huang, Shuai Yuan, Kun-Yu Wang, Bing-Han Li, Wan-Ling Liu, Gregory S. Day, Songsheng Tao, Chun-Chuen Yang, Tzuoo-Tsair Luo, Chia-Her Lin, Sue-Lein Wang, **Simon J. L. Billinge**, Kuang-Lieh Lu, Yves J. Chabal, Xiaodong Zou, and Hong-Cai Zhou. "Rapid desolvation-triggered domino lattice rearrangement in a metal–organic framework". In: *Nature Chemistry* 12 (2019), pp. 90–97. DOI: 10.1038/s41557-019-0364-0. URL: https://doi.org/10.1038/s41557-019-0364-0

27. Elizabeth A. Morrow, Maxwell W. Terban, Joo Won Lee, Leonard C. Thomas, **Simon J. L. Billinge**, and Shelly J. Schmidt. "Investigation of thermal decomposition as a critical factor inhibiting cold crystallization in amorphous sucrose prepared by melt-quenching: Effect of amorphization method on the physicochemical properties of amorphous sucrose". In: *J. Food Eng.*

261 (2019), pp. 87–99. DOI: 10.1016/j.jfoodeng.2019.05.026. URL: https://doi.org/10.1016/j.jfoodeng.2019.05.026

28. Aida Contreras-Ramirez, Songsheng Tao, Gregory S. Day, Vladimir I. Bakhmutov, **Simon J. L. Billinge**, and Hong-Cai Zhou. "Zirconium phosphate: the pathway from turbostratic disorder to crystallinity". In: *Inorganic Chemistry* 58.20 (2019), pp. 14260–14274. DOI: 10.1021/acs.inorgchem.9b02442. URL: https://pubs.acs.org/doi/full/10.1021/acs.inorgchem.9b02442

29. Soham Banerjee, Amirali Zangiabadi, Akbar Mahdavi-Shakib, Samra Husremovic, Brian G. Frederick, Katayun Barmak, Rachel Narehood Austin, and **Billinge, Simon J. L.** "Quantitative structural characterization of catalytically active TiO_2 nanoparticles". In: *ACS Appl. Nano Mater.* 2.10 (2019), pp. 6268–6276. DOI: 10.1021/acsanm.9b01246. URL: https://pubs.acs.org/doi/10.1021/acsanm.9b01246

30. **Billinge, S. J. L.** "Nanometre-scale structure from powder diffraction: total scattering and atomic pair distribution function analysis". In: *International Tables of Crystallography*. Ed. by Christopher Gilmore, James Kaduk, and Henk Schenk. Vol. H. Chester, UK: International Union of Crystallography, 2019. Chap. 5.7, pp. 649–672. DOI: 10.1107/97809553602060000972. URL: https://it.iucr.org/Ha/ch5o7v0001/

31. E. S. Bozin, W. G. Yin, R. J. Koch, M. Abeykoon, Y. S. Hor, H. Zheng, H. C. Lei, C. Petrovic, J. F. Mitchell, and **Billinge, S. J. L.** "Local orbital degeneracy lifting as a precursor to an orbital-selective Peierls transition". In: *Nature Commun.* 10 (2019), p. 3638. DOI: 10.1038/s41467-019-11372-w. URL: https://www.nature.com/articles/s41467-019-11372-w

32. Ran Gu, Soham Banerjee, Qiang Du, and **Billinge, Simon J. L.** "Algorithm for distance list extraction from pair distribution functions". In: *Acta Crystallogr. A* 75.5 (2019), pp. 658–668. DOI: 10.1107/S2053273319008647. URL: https://doi.org/10.1107/S2053273319008647

33. R. J. Koch, E. S. Bozin, C. Petrovic, Y. Zhu, M. Abeykoon, and **Billinge, Simon J. L.** "Room temperature local nematicity in an iron-selenide superconducing sample". In: *Phys. Rev. B., Rapid Communications* 100 (2019). Editor's suggestion, 020501(R). DOI: 10.1103/PhysRevB.100.020501. URL: https://journals.aps.org/prb/abstract/10.1103/PhysRevB.100.020501

34. Sandra H. Skjærvø, Quintin N. Meier, Mikhail Feygenson, Nicola A. Spaldin, **Simon J. L. Billinge**, Emil S. Bozin, and Sverre M. Selbach. "Unconventional order-disorder phase transition in improper ferroelectric hexagonal manganites". In: *Phys. Rev. X* 9 (2019), p. 031001. DOI: 10.1103/PhysRevX.9.031001. URL: https://journals.aps.org/prx/abstract/10.1103/PhysRevX.9.031001

35. Chia-Hao Liu, Yunzhe Tao, Daniel J. Hsu, Qiang Du, and **Billinge, Simon J. L.** "Using a machine learning approach to determine the space group of a structure from the atomic pair distribution function". In: *Acta Crystallogr. A* 75 (2019), pp. 633–643. DOI: 10.1107/S2053273319005606. URL: https://doi.org/10.1107/S2053273319005606

36. Xu Xiao, Hao Wang, Weizhai Bao, Patrick Urbankowski, Long Yang, Yao Yang, Kathleen Maleski, Linfan Cui, **Simon J. L. Billinge**, Guoxiu Wang, and Yury Gogotsi. "Two-dimensional arrays of transition metal nitride nanocrystals". In: *Adv. Mater.* 31.33 (2019), p. 02393. DOI: 10.1002/adma.201902393. URL: https://doi.org/10.1002/adma.201902393

37. T. Konstantinova, L. Wu, M. Abeykoon, R. J. Koch, A. F. Wang, R. K. Li, X. Shen, J. Li, J. Tao, I. A. Zaliznyak, C. Petrovic, **Billinge, S. J. L.**, X. J. Wang, E. S. Bozin, and Y. Zhu. "Photoinduced ultrafast dynamics of local nematicity and lattice distortions in FeSe crystals". In:

Phys. Rev. B, Rapid Communication. Editor's suggestion. 99 (2019), p. 180102. DOI: 10.1103/PhysRevB.99.180102. URL: https://journals.aps.org/prb/abstract/10.1103/PhysRevB.99.180102

38. Andy I. Nguyen, Kurt M. Van Allsburg, Maxwell W. Terban, Michal Bajdich, Julia Oktawiec, Jaruwan Amtawong, Micah S. Ziegler, James P. Dombrowski, K. V. Lakshmi, Walter S. Drisdell, Junko Yanoc, **Simon J. L. Billinge**, and T. Don Tilley. "Stabilization of reactive Co_4O_4 cubane oxygen-evolution catalysts within porous frameworks". In: *PNAS* 116 (2019), pp. 11630–11639. DOI: 10.1073/pnas.1815013116. URL: https://www.pnas.org/content/116/24/11630

39. **Billinge, Simon J. L.** "The rise of the x-ray atomic pair distribution function method: a series of fortunate events". In: *Philos T. Roy. Soc. A* 377 (2019), p. 20180413. DOI: 10.1098/rsta.2018.0413. URL: https://royalsocietypublishing.org/doi/10.1098/rsta.2018.0413

40. Alexander P. Aydt, Boyu Qie, Andrew Pinkard, Long Yang, Qian Cheng, **Billinge, Simon J. L.**, Yuan Yang, and Xavier Roy. "Microporous Battery Electrodes from Molecular Cluster Precursors". In: *ACS Appl. Mater. Interfaces* 11.12 (2019), pp. 11292–11297. DOI: 10.1021/acsami.8b18149. URL: https://pubs.acs.org/doi/abs/10.1021/acsami.8b18149

41. Xu Xiao, Patrick Urbankowski, Kanit Hantanasirisakul, Yao Yang, Stephen Sasaki, Long Yang, Chi Chen, Hao Wang, Ling Miao, Sarah H. Tolbert, **Billinge, Simon J. L.**, Hector D. Abruna, Steven J. May, and Yury Gogotsi. "Scalable synthesis of ultrathin Mn_3N_2 exhibiting room-temperature antiferromagnetism". In: *Adv. Funct. Mater.* (2019), p. 1809001. DOI: adfm.201809001. URL: https://onlinelibrary.wiley.com/doi/full/10.1002/adfm.201809001

42. Elizabeth A. Morrow, Maxwell W. Terban, Leonard C. Thomas, Danielle L. Gray, Michael J. Bowman, **Billinge, Simon J. L.**, and Shelly J. Schmidt. "Effect of amorphization method on the physicochemical properties of amorphous sucrose". In: *J. Food Eng.* 243 (2019), pp. 125–141. DOI: 10.1016/j.jfoodeng.2018.08.036. URL: https://www.sciencedirect.com/science/article/pii/S0260877418303790

43. Chenyang Shi, Alexander N. Beecher, Yan Li, Jonathan S. Owen, Bogdan M. Leu, Ayman H. Said, Michael Y. Hu, and **Billinge, Simon J. L.** "Size-dependent lattice dynamics of atomically precise cadmium selenide quantum dots". In: *Phys. Rev. Lett.* 122 (2019), p. 026101. DOI: 10.1103/PhysRevLett.122.026101. URL: https://journals-aps-org.ezproxy.cul.columbia.edu/prl/abstract/10.1103/PhysRevLett.122.026101

44. Julien Lombardi, Long Yang, Frederick A. Pearsall, Nasim Farahmand, Zheng Gai, **Billinge, Simon J. L.**, and Stephen O'Brien. "Stoichiometric control over ferroic behavior in $Ba(Ti_{1-x}Fe_x)O_3$ nanocrystals". In: *Chem. Mater.* 31.4 (2019), pp. 1318–1335. DOI: 10.1021/acs.chemmater.8b04447. URL: https://pubs.acs.org/doi/10.1021/acs.chemmater.8b04447

45. Parham Rohani, Soham Banerjee, Souroush Ashrafi-Asl, Mohammad Malekzadeh, Reza Shahbazian-Yassar, **Billinge, Simon J. L.**, and Mark T. Swihart. "Synthesis and properties of boron-hyperdoped silicon nanoparticles". In: *Adv. Funct. Mater.* (2019), p. 1807788. DOI: 10.1002/adfm.201807788. URL: https://onlinelibrary.wiley.com/doi/full/10.1002/adfm.201807788

46. **Billinge, Simon J. L.**, Philip M. Duxbury, Douglas S. Gonçalves, Carlile Lavor, and Antonio Mucherino. "Recent results on assigned and unassigned distance geometry with applications to protein molecules and nanostructures". In: *Ann. Oper. Res.* 271.1 (2018), 161–203. DOI: 10.1007/s10479-018-2989-6. URL: http://link.springer.com/article/10.1007/s10479-018-2989-6

47. Z. Guguchia, A. Kerelsky, D. Edelberg, S. Banerjee, F. von Rohr, D. Scullion, M. Augustin, M. Scully, Z. Shermadini, H. Luetkens, A. Shengelaya, C. Baines, E. Morenzoni, A. Amato, J. C. Hone, R. Khasanov, **Billinge, S. J. L.**, E. Santos, A. N. Pasupathy, and Y. J. Uemura. "Magnetism in Semiconducting Molybdenum Dichalcogenides". In: *Science Advances* 4 (2018), eaat3672. DOI: 10.1126/sciadv.aat3672. URL: https://advances.sciencemag.org/content/4/12/eaat3672

48. Wesley J. Transue, Matthew Nava, Maxwell W. Terban, Jing Yang, Matthew W. Greenberg, Gang Wu, Chantal L. Mustoe, Pierre Kennepohl, Jonathan S. Owen, **Billinge, Simon J. L.**, Heather J. Kulik, and Christopher C. Cummins. "Anthracene as a launchpad for a phosphinidene sulfide and for generation of a phosphorus–sulfur material having the composition P_2S, a vulcanized red phosphorus that is yellow". In: *J. Am. Chem. Soc.* 141 (2018), pp. 431–440. DOI: 10.1021/jacs.8b10775. URL: https://pubs.acs.org/doi/pdf/10.1021/jacs.8b10775

49. Soham Banerjee, Chia-Hao Liu, Jennifer D. Lee, Anton Kovyakh, Viktoria Grasmik, Oleg Prymak, Christopher Koenigsmann, Haiqing Liu, Lei Wang, A. M. Milinda Abeykoon, Stanislaus S. Wong, Matthias Epple, Christopher B. Murray, and **Billinge, Simon J. L.** "Improved models for metallic nanoparticle cores from atomic pair distribution function (PDF) analysis". In: *J. Phys. Chem. C* 122.51 (2018), pp. 29498–29506. DOI: 10.1021/acs.jpcc.8b05897. URL: https://pubs.acs.org/doi/10.1021/acs.jpcc.8b05897

50. Runze Yu, Emil S. Bozin, Milinda Abeykoon, Boris Sangiorgio, Nicola A. Spaldin, Christos D. Malliakas, Mercouri G. Kanatzidis, and **Billinge, Simon J. L.** "Emphanitic anharmonicity in PbSe at high temperature and the anomalous electronic properties in the PbX (X=S, Se, Te) system". In: *Phys. Rev. B* 98 (2018), p. 144108. DOI: 10.1103/PhysRevB.98.144108. URL: http://doi.org/10.1103/PhysRevB.98.144108

51. Yuguang C. Li, Elizabeth L. Melenbrink, Guy J. Cordonier, Christopher Boggs, Anupama Khan, Morko Kwembur Isaac, Lameck Kabambalika Nkhonjera, David Bahati, **Billinge, Simon J.**, Sossina M. Haile, Rodney A. Kreuter, Robert M. Crable, and Thomas E. Mallouk. "An easily fabricated low-cost potentiostat coupled with user- friendly software for introducing students to electrochemical reactions and electroanalytical techniques". In: *J. Chem. Educ.* 95 (2018), pp. 1658–1661. DOI: 10.1021/acs.jchemed.8b00340

52. Casey N. Brodsky, D. Kwabena Bediako, Chenyang Shi, Thomas Keane, Cyrille Costentin, **Billinge, Simon J. L.**, and Daniel G. Nocera. "Proton-electron conductivity in thin films of a cobalt-oxygen evolving catalyst". In: *ACS Appl. Energy Mater.* 2.1 (2018), pp. 3–12. DOI: 10.1021/acsaem.8b00785. URL: https://pubs.acs.org/doi/abs/10.1021/acsaem.8b00785

53. Pavol Juhás, Jaap N. Louwen, Lambert van Eijck, Eelco T. C. Vogt, and **Billinge, Simon J. L.** "*PDFgetN3*: atomic pair distribution functions from neutron powder diffraction data using *ad hoc* corrections". In: *J. Appl. Crystallogr.* 51.5 (2018), pp. 1492–1497. DOI: 10.1107/S1600576718010002. URL: https://doi.org/10.1107/S1600576718010002

54. Boris Sangiorgio, Emil S. Bozin, Christos D. Malliakas, Michael Fechner, Arkadiy Simonov, Mercouri G. Kanatzidis, **Billinge, Simon J. L.**, Nicola A. Spaldin, and Thomas Weber. "Correlated local dipoles in PbTe". In: *Phys. Rev. Materials* 2 (2018), p. 085402. DOI: 10.1103/PhysRevMaterials.2.085402. URL: https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.2.085402

55. Chenyang Shi, **Billinge, Simon J. L.**, Eric Puma, Sun Hwi Bang, Nathaniel J. H. Bean, Jean-Claude de Sugny, Robert G. Gambee, Richard C. Haskell, Adrian Hightower, and Todd C. Monson. "Barium titanate nanoparticles: short-range lattice distortions with long-range

cubic order". In: *Phys. Rev. B* 98 (2018), p. 085421. DOI: 10.1103/PhysRevB.98.085421. URL: https://doi.org/10.1103/PhysRevB.98.085421

56. Hannes Rijckaert, Jonathan De Roo, Matthias Van Zele, Soham Banerjee, Hannu Huhtinen, Petriina Paturi, Jan Bennewitz, **Billinge, Simon J. L.**, Michael Bäcker, Klaartje De Buysser, and Isabel Van Driessche. "Pair distribution function analysis of ZrO_2 Nanocrystals and insights in the formation of ZrO_2-$YBa_2Cu_3O_7$ nanocomposites". In: *MDPI-Materials* 11 (2018), p. 1066. DOI: 10.3390/ma11071066. URL: https://www.mdpi.com/1996-1944/11/7/1066

57. James Gong and **Billinge, Simon J. L.** "Atomic pair distribution functions (PDFs) from textured polycrystalline samples: fundamentals". In: (2018). arXiv:1805.10342 [cond-mat.mtrl-sci]. URL: https://arxiv.org/abs/1805.10342

58. Boyuan Zhang, Raúl H. Sánchez, Yu Zhong, Melissa Ball, Maxwell W. Terban, Daniel Paley, **Billinge, Simon J. L.**, Fay Ng, Michael L. Steigerwald, and Colin Nuckolls. "Hollow organic capsules assemble into cellular semiconductors". In: *Nat. Commun.* 9 (2018), p. 1957. DOI: 10.1038/s41467-018-04246-0. URL: https://www.nature.com/articles/s41467-018-04246-0

59. Federica Bertolotti, Andrew H. Proppe, Dmitry N. Dirin, Mengxia Liu, Oleksandr Voznyy, Antonio Cervellino, **Billinge, Simon J. L.**, Maksym V. Kovalenko, Edward H. Sargent, Norberto Masciocchi, and Antonietta Guagliardi. "Ligand-induced symmetry breaking, size and morphology in colloidal lead sulfide QDs: from classic to thiourea precursors". In: *Chem2* 2.1 (2018). DOI:10.28954/2018.csq.02.001, p. 1. DOI: 10.28954/2018.csq.02.001. URL: http://doi.org/10.28954/2018.csq.02.001

60. Maxwell W. Terban, Debasis Banerjee, Sanjit Ghose, Bharat Medasani, Anil Shukla, Benjamin A. Legg, Yufan Zhou, Zihua Zhu, Maria L. Sushko, Jim J. De Yoreo, Jun Liu, Praveen K. Thallapally, and **Billinge, Simon J. L.** "Early stage structural development of prototypical zeolitic imidazolate framework (ZIF) in solution". In: *Nanoscale* 10 (2018), pp. 4291–4300. DOI: 10.1039/C7NR07949D. URL: http://pubs.rsc.org/en/content/articlelanding/2018/nr/c7nr07949d/unauth\#!divAbstract

61. Benjamin A. Frandsen, Kathryn A. Ross, Jason W. Krizan, Gøran J. Nilsen, Andrew R. Wildes, Robert J. Cava, Robert J. Birgeneau, and **Billinge, Simon J. L.** "Real-space investigation of short-range magnetic correlations in fluoride pyrochlores $NaCaCo_2F_7$ and $NaSrCo_2F_7$ with magnetic pair distribution function analysis". In: *Phys. Rev. Materials* 1 (2017). Selected as Editor's Choice, p. 074412. DOI: 10.1103/PhysRevMaterials.1.074412. URL: https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.1.074412

62. Josefa Vidal Laveda, Beth Johnston, Gary W. Paterson, Peter J. Baker, Matthew G. Tucker, Helen Y. Playford, Kirsten M. Ø. Jensen, **Billinge, Simon J. L.**, and Serena A. Corr. "Structure-property insights into nanostructured electrodes for Li-ion batteries from local structural and diffusional probes". In: *J. Mater. Chem. A* 6 (2017), p. 127. DOI: 10.1039/c7ta04400c. URL: http://doi.org/10.1039/c7ta04400c

63. Crystal S. Lewis, Dominic Moronta, Maxwell W. Terban, Lei Wang, Shiyu Yue, Cheng Zhang, Qiang Li, Adam Corrao, **Billinge, Simon J. L.**, and Stanislaus S. Wong. "Synthesis, characterization, and growth mechanism of motifs of ultrathin cobalt-substituted $NaFeSi_2O_6$ nanowires". In: *CrystEngComm* 20 (2017). art, typeB1, fy18, pp. 223–236. DOI: 10.1039/C7CE01885A. URL: http://pubs.rsc.org/-/content/articlehtml/2018/ce/c7ce01885a

64. Patrick Urbankowski, Babak Anasori, Kanit Hantanasirisakul, Long Yang, Lihua Zhang, Bernard Haines, Steven J. May, **Billinge, Simon J. L.**, and Yury Gogotsi. "2D molybdenum and

vanadium nitrides synthesized by ammoniation of 2D transition metal carbides (MXenes)". In: *Nanoscale* 9 (2017), pp. 17722–17730. DOI: 10.1039/C7NR06721F. URL: http://pubs.rsc.org/en/content/articlehtml/2017/nr/c7nr06721f

65. Z. Guguchia, T. Adachi, Z. Shermadini, T. Ohgi, J. Chang, E. Bozin, F. von Rohr, A. M. dos Santos, J. J. Molaison, Y. Koike, A. R. Wieteska, B. A. Frandsen, E. Morenzoni, A. Amato, **Billinge, S. J. L.**, Y. J. Uemura, and R. Khasanov. "Pressure tuning of structure, superconductivity and novel magnetic order in the Ce-underdoped electron-doped cuprate T′-$Pr_{1.3-x}La_{0.7}Ce_xCuO_4$ ($x = 0.1$)". In: *Phys. Rev. B* 96 (2017), p. 094515. DOI: 10.1103/PhysRevB.96.094515. URL: https://journals.aps.org/prb/abstract/10.1103/PhysRevB.96.094515

66. Nathan Nakamura, Maxwell W. Terban, **Billinge, Simon J. L.**, and B. Reeja Jayan. "Unlocking the structure of mixed amorphous-crystalline ceramic oxide films synthesized under low temperature electromagnetic excitation". In: *J. Mater. Chem. A* 5.35 (2017), pp. 18434–18441. DOI: 10.1039/C7TA06339C. URL: pubs.rsc.org/en/content/articlehtml/2017/ta/c7ta06339c

67. Jennifer L. Stein, Molly I. Steimle, Maxwell W. Terban, Alessio Petrone, **Billinge, Simon J. L.**, Xiaosong Li, and Brandi M. Cossairt. "Cation exchange induced transformation of InP magic-sized clusters". In: *Chem. Mater.* 29.18 (2017), pp. 7984–7992. DOI: 10.1021/acs.chemmater.7b03075. URL: pubs.acs.org/doi/abs/10.1021/acs.chemmater.7b03075

68. Maxwell W. Terban, Chenyang Shi, Rita Silbernagel, Abraham Clearfield, and **Billinge, Simon J. L.** "Local environment of terbium(III) ions in layered nanocrystalline zirconium(IV) phosphonate–phosphate ion exchange materials". In: *Inorg. Chem.* 56.15 (2017), pp. 8837–8846. DOI: 10.1021/acs.inorgchem.7b00666. URL: http://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.7b00666

69. Federica Bertolotti, Loredana Protesescu, Maksym V. Kovalenko, Sergii Yakunin, Antonio Cervellino, **Billinge, Simon J. L.**, Maxwell W. Terban, Jan Skov Pedersen, Norberto Masciocchi, and Antonietta Guagliardi. "Coherent nanotwins and dynamic disorder in cesium lead halide perovskite nanocrystals". In: *ACS Nano.* 11 (2017), pp. 3819–3831. DOI: 10.1021/acsnano.7b00017. URL: http://pubs.acs.org/doi/abs/10.1021/acsnano.7b00017

70. Liliana Gamez, Maxwell W. Terban, **Billinge, Simon J. L.**, and Maria Martinez-Inesta. "Modelling and validation of particle size distributions of supported nanoparticles using the pair distribution function technique". In: *J. Appl. Crystallogr.* 50.3 (2017), pp. 741–748. DOI: 10.1107/S1600576717003715. URL: http://scripts.iucr.org/cgi-bin/paper?S1600576717003715

71. Lijun Li, Xiaoyu Deng, Zhen Wang, Yu Liu, Milinda Abeykoon, Eric Dooryhee, Aleksandra Tomic, Yanan Huang, John B. Warren, Emil S. Bozin, **Billinge, Simon J. L.**, Yuping Sun, Yimei Zhu, Gabriel Kotliar, and Cedomir Petrovic. "Superconducting order from disorder in 2H-$TaSe_{2-x}S_x$". In: *npj Quantum Mater.* 2 (2017), p. 11. DOI: 10.1038/s41535-017-0016-9. URL: http://www.nature.com/articles/s41535-017-0016-9?WT.ec_id=NPJQUANTMATS-201702&spMailingID=53494924&spUserID=MjE2OTY3OTY1OTA3S0&spJobID=1103960492&spReportId=MTEwMzk2MDQ5MgS2

72. Z. Guguchia, F. von Rohr, Z. Shermadini, A. T. Lee, S. Banerjee, A. R. Wieteska, C. A. Marianetti, B. A. Frandsen, H. Luetkens, Z. Gong, S. C. Cheung, C. Baines, A. Shengelaya, G. Taniashvili, A. N. Pasupathy, E. Morenzoni, **Billinge, S. J. L.**, A. Amato, R. J. Cava, R. Khasanov, and Y. J. Uemura. "Signatures of the topological s^{+-} superconducting order parameter in the type-II Weyl semimetal T_d-$MoTe_2$". In: *Nat. Commun.* 8 (2017), p. 1082. DOI: 10.1038/s41467-017-01066-6. URL: https://www.nature.com/articles/s41467-017-01066-6

73. **Billinge, Simon J. L.**, Philip M. Duxbury, Douglas S. Gonçalves, Carlile Lavor, and Antonio Mucherino. "Assigned and unassigned Distance Geometry: applications to Biological Molecules and Nanostructures". In: *4OR-Q J Oper Res* 14 (2016), pp. 337–376. DOI: 10.1007/s10288-016-0314-2. URL: http://link.springer.com/article/10.1007/s10288-016-0314-2

74. Z. Guguchia, R. Khasanov, A. Shengelaya, E. Pomjakushina, **Billinge, S. J. L.**, A. Amato, E. Morenzoni, and H. Keller. "Cooperative coupling of static magnetism and bulk superconductivity in the stripe phase of $La_{2-x}Ba_xCuO_4$: Pressure- and doping-dependent studies". In: *Phys. Rev. B* 94 (2016), p. 214511. DOI: 10.1103/PhysRevB.94.214511. URL: https://journals.aps.org/prb/abstract/10.1103/PhysRevB.94.214511

75. Ann-Christin Dippel, Kirsten M. Ø. Jensen, Christoffer Tyrsted, Martin Bremholm, Espen D. Bøjesen, Dipankar Saha, Steinar Birgisson, Mogens Christensen, **Billinge, Simon J. L.**, and Bo B. Iversen. "Towards atomistic understanding of polymorphism in solvothermal synthesis of ZrO_2 nanoparticles". In: *Acta Crystallogr. A* 72 (2016), pp. 645–650. DOI: 10.1107/S2053273316012675. URL: http://scripts.iucr.org/cgi-bin/paper?S2053273316012675

76. Paolo Scardi, **Billinge, Simon J. L.**, Reinhard Neder, and Antonio Cervellino. "Celebrating 100 years of the Debye scattering equation". In: *Acta Crystallogr. A* 72 (2016), pp. 589–590. DOI: 10.1107/S2053273316015680. URL: http://scripts.iucr.org/cgi-bin/paper?S2053273316015680

77. 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 **Billinge, Simon J. L.** "Direct observation of dynamic symmetry breaking above room temperature in methylammonium lead iodide perovskite". In: *ACS Energy Lett.* 1.4 (2016), 880–887. DOI: 10.1021/acsenergylett.6b00381. URL: http://dx.doi.org/10.1021/acsenergylett.6b00381

78. **Billinge, Simon J. L.** "Physics inside: solving protein structures without crystals". In: *Condensed Matter Physics Journal Club* (2016). URL: http://www.condmatjournalclub.org/?p=2913

79. Benjamin A. Frandsen, Zizhou Gong, Maxwell W. Terban, Soham Banerjee, Bijuan Chen, Changqing Jin, Mikhail Feygenson, Yasutomo J. Uemura, and **Billinge, Simon J. L.** "Local atomic and magnetic structure of dilute magnetic semiconductor $(Ba,K)(Zn,Mn)_2As_2$". In: *Phys. Rev. B* 94 (2016). selected as Editors' Suggestion, p. 094102. DOI: 10.1103/PhysRevB.94.094102. URL: https://doi.org/10.1103/PhysRevB.94.094102

80. Jianwei Miao, Peter Ercius, and **Billinge, Simon J. L.** "Atomic electron tomography: 3D structures without crystals". In: *Science* 353.6306 (2016), aaf2157. DOI: 10.1126/science.aaf2157. URL: http://science.sciencemag.org/content/353/6306/aaf2157

81. Maxwell W. Terban, Raphaël Dabbous, Anthony D. Debellis, Elmar Pöselt, and **Billinge, Simon J. L.** "Structures of hard phases in thermoplastic polyurethanes". In: *Macromolecules* 49.19 (2016), pp. 7350–7358. DOI: 10.1021/acs.macromol.6b00889. URL: http://pubs.acs.org/doi/abs/10.1021/acs.macromol.6b00889

82. Benjamin A. Frandsen, Lian Liu, Sky C. Cheung, Zurab Guguchia, Rustem Khasanov, Elvezio Morenzoni, Timothy J. S. Munsie, Alannah M. Hallas, Murray N. Wilson, Yipeng Cai, Graeme M. Luke, Bijuan Chen, Wenmin Li, Changqing Jin, Cui Ding, Shengli Guo, Fanlong Ning, Takashi Ito, Wataru Higemoto, **Billinge, Simon J. L.**, Shoya Sakamoto, Atsushi Fujimori, Taito Murakami, Hiroshi Kageyama, Jose Antonio Alonso, Gabriel Kotliar, Masatoshi Imada, and

Yasuotomo J. Uemura. "Volume-wise destruction of the antiferromagnetic Mott insulating state through quantum tuning". In: *Nat. Commun.* 7 (2016), p. 12519. DOI: 10.1038/ncomms12519. URL: http://www.nature.com/articles/ncomms12519

83. E. S. Bozin and **Billinge, S. J. L.** "Novel trends in pair distribution function approaches on bulk systems with nanoscale heterogeneities". In: *Neutron News* 27.3 (2016), pp. 27–31. DOI: 10.1080/10448632.2016.1197602. URL: http://dx.doi.org/10.1080/10448632.2016.1197602

84. Benjamin A. Frandsen and **Billinge, Simon J. L.** "Investigating short-range magnetic correlations in real space with the magnetic pair distribution function (mPDF)". in: *Neutron News* 27 (3 2016), pp. 14–16. DOI: 10.1080/10448632.2016.1197588. URL: http://www.tandfonline.com/doi/full/10.1080/10448632.2016.1197588

85. Kirsten M. Ø. Jensen, Pavol Juhás, Marcus A. Tofanelli, Christine L. Heinecke, Gavin Vaughan, Christopher J. Ackerson, and **Billinge, Simon J. L.** "Polymorphism in magic sized $Au_{144}(SR)_{60}$ clusters". In: *Nat. Commun.* 7 (2016), p. 11859. DOI: 10.1038/ncomms11859. URL: http://dx.doi.org/10.1038/ncomms11859

86. P. M. Duxbury, L. Granlund, S. R. Gujarathi, P. Juhás, and **Billinge, Simon J. L.** "The unassigned distance geometry problem". In: *Discrete Applied Mathematics* 204 (2016), pp. 117–132. DOI: 10.1016/j.dam.2015.10.029. URL: http://www.sciencedirect.com/science/article/pii/S0166218X15005168

87. Benjamin A. Frandsen, Michela Brunelli, Katherine Page, Yasutomo J. Uemura, Julie B. Staunton, and **Billinge, Simon J. L.** "Verification of Anderson Superexchange in MnO via Magnetic Pair Distribution Function Analysis and *ab initio* Theory". In: *Phys. Rev. Lett.* 116 (19 2016), p. 197204. DOI: 10.1103/PhysRevLett.116.197204. URL: http://link.aps.org/doi/10.1103/PhysRevLett.116.197204

88. Mouath Shatnawi, Emil S. Bozin, J. F. Mitchell, and **Billinge, Simon J. L.** "Non percolative nature of the metal-insulator transition and persistence of local Jahn-Teller distortions in the rhombohedral regime of $La_{1-x}Ca_xMnO_3$". In: *Phys. Rev. B* 93 (2016), p. 165138. DOI: 10.1103/PhysRevB.93.165138. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.93.165138

89. J. Choi and **Billinge, S. J. L.** "Perovskites at the nanoscale: from fundamentals to applications". In: *Nanoscale* 8 (2016), pp. 6206–6208. DOI: 10.1039/C6NR90040B. URL: http://pubs.rsc.org/en/Content/ArticleLanding/2016/NR/C6NR90040B

90. Philip M. Duxbury and **Billinge, Simon J. L.** "Graph rigidity, unassigned distance geometry and the nanostructure problem". In: *Signals, Systems and Computers, 2016 50th Asilomar Conference*. Ed. by Michael B. Matthews. IEEE, 2016, pp. 1483–1487. DOI: 10.1109/ACSSC.2016.7869624. URL: http://ieeexplore.ieee.org/abstract/document/7869624/

91. Babak Anasori, Chenyang Shi, Eun Ju Moon, Yu Xie, Cooper A. Voigt, Paul R. C. Kent, Steven J. May, **Billinge, Simon J. L.**, Michel W. Barsoum, and Yury Gogotsi. "Control of electronic properties of 2D carbides (MXenes) by manipulating their transition metal layers". In: *Nanoscale Horiz.* 1.3 (2016), pp. 227–234. DOI: 10.1039/C5NH00125K. URL: http://pubs.rsc.org/is/content/articlelanding/2016/nh/c5nh00125k/

92. Dragica Prill, Pavol Juhás, **Billinge, S. J. L.**, and Martin U. Schmidt. "Towards solution and refinement of organic crystal structures by fitting to the atomic pair distribution function". In: *Acta Crystallogr. A* 72.1 (2016), pp. 62–72. DOI: 10.1107/S2053273315022457. URL: http://scripts.iucr.org/cgi-bin/paper?S2053273315022457

93. Pavol Juhás, Christopher L. Farrow, Xiaohao Yang, Kevin R. Knox, and **Billinge, Simon J. L.** "Complex Modeling: a strategy and software program for combining multiple information sources to solve ill-posed structure and nanostructure inverse problems". In: *Acta Crystallogr. A* 71.6 (2015), pp. 562–568. DOI: 10.1107/S2053273315014473. URL: http://dx.doi.org/10.1107/S2053273315014473

94. Dragica Prill, Pavol Juhás, Martin U. Schmidt, and **Billinge, Simon J. L.** "Modeling pair distribution functions (PDF) of organic compounds: describing both intra- and intermolecular correlation functions in calculated PDFs". In: *J. Appl. Crystallogr.* 48.1 (2015), pp. 171–178. DOI: 10.1107/S1600576714026454. URL: http://dx.doi.org/10.1107/S1600576714026454

95. Maxwell W. Terban, Matthew Johnson, Marco DiMichiel, and **Billinge, Simon J. L.** "Detection and characterization of nanoparticles in suspension at low concentrations using the x-ray total scattering pair distribution function technique". In: *Nanoscale* 7 (2015), pp. 5480–5487. DOI: 10.1039/C4NR06486K. URL: http://dx.doi.org/10.1039/C4NR06486K

96. Milinda Abeykoon, Hefei Hu, Lijun Wu, Yimei Zhu, and **Billinge, Simon J. L.** "Calibration and data collection protocols for reliable lattice parameter values in electron pair distribution function studies". In: *J. Appl. Crystallogr.* 48 (2015), pp. 244–251. DOI: 10.1107/S1600576715000412. URL: http://journals.iucr.org/j/issues/2015/01/00/po5013/po5013.pdf

97. **Billinge, Simon J. L.** and Jianwei Miao. "Celebrating the past, looking to the future". In: *Acta Crystallogr. A* 71 (2015), pp. 1–2. DOI: 10.1107/S2053273314027685. URL: http://dx.doi.org/10.1107/S2053273314027685

98. **Billinge, Simon J. L.** "Atomic pair distribution function: a revolution in the characterization of nanostructured pharmaceuticals". In: *Nanomedicine* 10.16 (2015), pp. 2473–2475. DOI: 10.2217/NNM.15.116. URL: http://www.futuremedicine.com/doi/abs/10.2217/nnm.15.116

99. E. S. Bozin, R. Zhong, K. R. Knox, G. Gu, J. P. Hill, J. M. Tranquada, and **Billinge, S. J. L.** "Reconciliation of local and long-range tilt correlations in underdoped $La_{2-x}Ba_xCuO_4$ ($0 \leq x \leq 0.155$)". In: *Phys. Rev. B* 91.5 (2015), p. 054521. DOI: 10.1103/PhysRevB.91.054521. URL: http://link.aps.org/doi/10.1103/PhysRevB.91.054521

100. Benjamin A. Frandsen and **Billinge, Simon J. L.** "Magnetic structure determination from the magnetic pair distribution function (mPDF): ground state of MnO". in: *Acta Crystallogr. A* 71.3 (2015), pp. 325–334. DOI: 10.1107/S205327331500306X. URL: http://journals.iucr.org/a/issues/2015/03/00/vk5003/index.html

101. Dylan C. Gary, Maxwell Terban, **Billinge, Simon J. L.**, and Brandi M. Cossairt. "Two-step nucleation and growth of InP quantum dots via magic-sized cluster intermediates". In: *Chem. Mater.* 27.4 (2015), pp. 1432–1441. DOI: 10.1021/acs.chemmater.5b00286. URL: http://pubs.acs.org/doi/abs/10.1021/acs.chemmater.5b00286

102. Tatiana E. Gorelik, Martin U. Schmidt, Ute Kolb, and **Billinge, Simon J. L.** "Total-Scattering Pair-Distribution-Function of Organic Material from Powder Electron Diffraction Data". In: *Microsc. Microanal.* 21 (2015), pp. 459 –471. DOI: 10.1017/S1431927614014561. URL: http://journals.cambridge.org/article_S1431927614014561

103. L. Granlund, **Billinge, S. J. L.**, and P. M. Duxbury. "Algorithm for systematic peak extraction from atomic pair distribution functions". In: *Acta Crystallogr. A* 71.4 (2015), pp. 392–409. DOI: 10.1107/S2053273315005276. URL: https://dx.doi.org/10.1107/S2053273315005276

104. Jessica M. Hudspeth, Tapan Chatterji, **Billinge, Simon J. L.**, and Simon A. J. Kimber. "Unifying local and average structure in the phase change material GeTe". In: *arXiv* (2015). 1506.08944 [cond-mat.mtrl-sci]. URL: http://arxiv.org/abs/1506.08944

105. Michael Huynh, Chenyang Shi, **Billinge, Simon J. L.**, and Daniel Nocera. "Nature of activated manganese oxide for oxygen evolution". In: *J. Am. Chem. Soc.* 137 (2015), 14887–14904. DOI: 10.1021/jacs.5b06382. URL: https://pubs.acs.org/doi/pdf/10.1021/jacs.5b06382

106. Kirsten M. Ø. Jensen, Anders B. Blichfeld, Sage R. Bauers, Suzannah R. Wood, Eric Dooryhée, David C. Johnson, Bo B. Iversen, and **Billinge, Simon J. L.** "Demonstration of thin film pair distribution function analysis (tfPDF) for the study of local structure in amorphous and crystalline thin films". In: *IUCrJ.* 2.5 (2015), pp. 481–489. DOI: 10.1107/S2052252515012221. URL: http://journals.iucr.org/m/issues/2015/05/00/yu5008/

107. Kirsten M. Ø. Jensen, Xiaohao Yang, Josefa Vidal Laved, Wolfgang G. Zeir, Kimberly A. See, Marco DiMichiel, Brent C. Melot, Serena A. Corr, and **Billinge, Simon J. L.** "X-ray diffraction computed tomography for structural analysis of electrode materials in batteries". In: *J. Electrochem. Soc.* 162.7 (2015), A1310–A1314. DOI: 10.1149/2.0771507jes. URL: http://jes.ecsdl.org/content/162/7/A1310.abstract

108. S. Lendinez, R. Zarzuela, J. Tejada, M. W. Terban, **Billinge, S. J. L.**, J. Espin, I. Imaz, D. Maspoch, and E. M. Chudnovsky. "Resonant spin tunneling in randomly oriented nanospheres of Mn 12 acetate". In: *Phys. Rev. B* 91.2 (2015), p. 024404. DOI: 10.1103/PhysRevB.91.024404. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.91.024404

109. Maxwell W. Terban, Eugene Y. Cheung, Paul Krolikowski, and **Billinge, Simon J. L.** "Recrystallization, phase composition, and local structure of amorphous lactose from the total scattering pair distribution function". In: *Cryst. Growth Des.* 16.1 (2015), 210–220. DOI: 10.1021/acs.cgd.5b01100. URL: http://pubs.acs.org/doi/full/10.1021/acs.cgd.5b01100

110. Amanda L. Tiano, Georgia C. Papaefthymiou, Crystal S. Lewis, Jinkyu Han, Cheng Zhang, Qiang Li, Chenyang Shi, A. M. Milinda Abeykoon, **Billinge, Simon J. L.**, Eric Stach, Justin Thomas, Kevin Guerrero, Pablo Munayco, Jimmy Munayco, Rosa B. Scorzelli, Philip Burnham, Arthur J. Viescas, and Stanislaus S. Wong. "Correlating size and composition-dependent effects with magnetic, Mössbauer, and pair distribution function measurements in a family of catalytically active ferrite nanoparticles". In: *Chem. Mater.* 27 (2015), pp. 3572–3592. DOI: 10.1021/acs.chemmmater.5b00767. URL: http://pubs.acs.org/doi/abs/10.1021/acs.chemmater.5b00767

111. Kefeng Wang, Aifeng Wang, A. Tomic, Limin Wang, A. M. Milinda Abeykoon, E. Dooryhee, **Billinge, S. J. L.**, and C. Petrovic. "Enhanced thermoelectric power and electronic correlations in $RuSe_2$". In: *APL Mat.* 3 (2015), p. 041513. DOI: 10.1063/1.4913919. URL: http://dx.doi.org/10.1063/1.4913919

112. Xiaohao Yang, Pavol Juhás, Christopher Farrow, and **Billinge, Simon J. L.** "xPDFsuite: an end-to-end software solution for high throughput pair distribution function transformation, visualization and analysis". In: *arXiv* (2015). 1402.3163. URL: http://arxiv.org/abs/1402.3163

113. Alexander N. Beecher, Xiaohao Yang, Joshua H. Palmer, Alexandra L. LaGrassa, Pavol Juhás, **Billinge, Simon J. L.**, and Jonathan S. Owen. "Atomic structures and gram scale synthesis of three tetrahedral quantum dots". In: *J. Am. Chem. Soc.* 136.30 (2014), pp. 10645–10653. DOI: 10.1021/ja503590h. URL: http://pubs.acs.org/doi/abs/10.1021/ja503590h

114. E. S. Božin, K. R. Knox, P. Juhás, Y. S. Hor, J. F. Mitchell, and **Billinge, S. J. L.** "$Cu(Ir_{1-x}Cr_x)_2S_4$: a model system for studying nanoscale phase coexistence at the metal-insulator transition". In: *Sci. Rep.* 4 (2014), p. 4081. DOI: 10.1038/srep04081. URL: http://www.nature.com/srep/2014/140212/srep04081/full/srep04081.html

115. F. Bridges, T. Keiber, P. Juhás, **Billinge, S. J. L.**, L. Sutton, J. Wilde, and G. R. Kowach. "Local vibrations and negative thermal expansion in ZrW_2O_8". In: *Phys. Rev. Lett.* 112 (2014), p. 045505. DOI: 10.1103/PhysRevLett.112.045505. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.112.045505

116. Joshua J. Choi, Xiaohao Yang, Zachariah M. Norman, **Billinge, Simon J. L.**, and Jonathan S. Owen. "Structure of methylammonium lead iodide on mesoporous titanium dioxide: active material in high performance metal-organic solar cells". In: *Nano Lett.* 14.1 (2014), 127–133. DOI: 10.1021/nl403514x. URL: http://pubs.acs.org/doi/abs/10.1021/nl403514x

117. Vicky V. T. Doan-Nguyen, Simon A. J. Kimber, Diego Pontoni, Danielle Reifsnyder Hickey, Benjamin T. Diroll, Xiaohao Yang, Marcel Miglierini, Christopher B. Murray, and **Billinge, Simon J. L.** "Bulk metallic glass-like scattering signal in small metallic nanoparticles". In: *ACS Nano.* 8.6 (2014), pp. 6163–6170. DOI: 10.1021/nn501591g. URL: http://dx.doi.org/10.1021/nn501591g

118. Christoper L. Farrow, Chenyang Shi, Pavol Juhás, Xiaogang Peng, and **Billinge, Simon J. L.** "Robust structure and morphology parameters for CdS nanoparticles by combining small angle X-ray scattering and atomic pair distribution function data in a complex modeling framework". In: *J. Appl. Crystallogr.* 47 (2014), pp. 561–565. DOI: 10.1107/S1600576713034055. URL: http://journals.iucr.org/j/issues/2014/02/00/issconts.html

119. Benjamin A. Frandsen, Xiaohao Yang, and **Billinge, Simon J. L.** "Magnetic pair distribution function analysis of local magnetic correlations". In: *Acta Crystallogr. A* 70.1 (2014), pp. 3–11. DOI: 10.1107/S2053273313033081. URL: http://journals.iucr.org/a/issues/2014/01/00/mq5020/index.html

120. Benjamin A. Frandsen, Emil S. Bozin, Hefei Hu, Yimei Zhu, Yasumasa Nozaki, Hiroshi Kageyama, Yasutomo J. Uemura, Wei-Guo Yin, and **Billinge, Simon J. L.** "Intra-unit-cell nematic charge order in the titanium-oxypnictide family of superconductors". In: *Nat. Commun.* 5 (2014), p. 5761. DOI: 10.1038/ncomms6761. URL: http://www.nature.com/ncomms/2014/141208/ncomms6761/full/ncomms6761.html

121. Michael Ghidiu, Michael Naguib, Chenyang Shi, Olha Mashtalir, Limei Pan, Bo Zhang, Jian Yang, Yury Gogotsi, **Billinge, Simon J. L.**, and Michel W. Barsoum. "Synthesis and charaterization of two-dimensional Nb_4C_3 (MXene)". In: *Chem. Commun.* 50 (2014), pp. 9517–9520. DOI: 10.1039/c4cc03366c. URL: http://pubs.rsc.org/en/content/articlelanding/2014/cc/c4cc03366c\#!divAbstract

122. Hefei Hu, Yimei Zhu, Xiaoya Shi, Qiang Li, Ruidan Zhong, John A. Schneeloch, Genda Gu, John M. Tranquada, and **Billinge, Simon J. L.** "Nanoscale coherent intergrowth-like defects in a crystal of made superconducting by high-pressure oxygen annealing $La_{1.9}Ca_{1.1}Cu_2O_{6+\delta}$". In: *Phys. Rev. B* 90 (2014), p. 134518. DOI: 10.1103/PhysRevB.90.134518. URL: http://link.aps.org/doi/10.1103/PhysRevB.90.134518

123. Kirsten M. Ø. Jensen, Henrik L. Andersen, Christoffer Tyrsted, Espen D. Bojesen, Ann-Christin Dippel, Nina Lock, **Billinge, Simon J. L.**, Bo B. Iversen, and Mogens Christensen. "Mechanisms for iron oxide formation under hydrothermal conditions: an in situ total scattering study". In: *ACS Nano.* 8.10 (2014), 10704–10714. DOI: 10.1021/nn5044096. URL: http://pubs.acs.org/doi/abs/10.1021/nn5044096

124. K. R. Knox, E. S. Bozin, C. D. Malliakas, M. G. Kanatzidis, and **Billinge, S. J. L.** "Local off-centering symmetry breaking in the high temperature regime of SnTe". In: *Phys. Rev. B* 89 (1 2014), p. 014102. DOI: 10.1103/PhysRevB.89.014102. URL: http://link.aps.org/doi/10.1103/PhysRevB.89.014102

125. Shuangyi Liu, Andrew R. Akbashev, Xiaohao Yang, Xiaohua Liu, Wanlu Li, Lukas Zhao, Xue Li, Alexander Couzis, Myung-Geun Han, Yimei Zhu, Lia Krusin-Elbaum, Jackie Li, Limin Huang, **Billinge, Simon J. L.**, Jonathan E. Spanier, and Stephen O'Brien. "Hollandites as a new class of multiferroics". In: *Sci. Rep.* 4 (2014), p. 6203. DOI: 10.1038/srep06203. URL: http://www.nature.com/srep/2014/140827/srep06203/full/srep06203.html

126. Chenyang Shi, Majid Beidaghi, Michael Naguib, Olha Mashtalir, Yury Gogotsi, and **Billinge, Simon J. L.** "Structure of nanocrystalline Ti_3C_2 MXene using atomic pair distribution function". In: *Phys. Rev. Lett.* 112 (2014), p. 125501. DOI: 10.1103/PhysRevLett.112.125501. URL: http://link.aps.org/doi/10.1103/PhysRevLett.112.125501

127. Christoffer Tyrsted, Nina Lock, Kirsten M. Ø. Jensen, Mogens Christensen, Espen D. Bøjesen, Hermann Emerich, Gavin Vaughan, **Billinge, Simon J. L.**, and Bo B. Iversen. "Evolution of atomic structure during nanoparticle synthesis". In: *IUCrJ.* 1.3 (2014), pp. 165–171. DOI: 10.1107/S2052252514006538. URL: http://journals.iucr.org/m/issues/2014/03/00/fc5001/

128. Xiaohao Yang, P. Juhás, and **Billinge, S. J. L.** "On the estimation of statistical uncertainties on powder diffraction and small-angle scattering data from two-dimensional X-ray detectors". In: *J. Appl. Crystallogr.* 47.4 (2014), pp. 1273–1283. DOI: 10.1107/S1600576714010516. URL: http://journals.iucr.org/j/issues/2014/04/00/nb5095/

129. Mengqiang Zhu, Paul Northrup, Chenyang Shi, **Billinge, Simon J. L.**, Donald L. Sparks, and Glenn A. Waychunas. "The structure of sulfate adsorption complexes on ferrihydrite". In: *Environ. Sci. Technol. Lett.* 1 (2014), pp. 97–101. DOI: 10.1021/ez400052r. URL: http://pubs.acs.org/doi/abs/10.1021/ez400052r

130. K. R. Knox, A. M. M. Abeykoon, H. Zheng, W. G. Yin, A. M. Tsvelik, J. F. Mitchell, **Billinge, S. J. L.**, and E. S. Bozin. "Local structural evidence for strong electronic correlations in spinel $LiRh_2O_4$". In: *Phys. Rev. B* 88 (17 2013), p. 174114. DOI: 10.1103/PhysRevB.88.174114. URL: http://link.aps.org/doi/10.1103/PhysRevB.88.174114

131. Milinda Abeykoon, Emil S. Bozin, Genda Gu, John Hill, John Tranquada, and **Billinge, Simon J. L.** "Evidence for short-range-ordered charge stripes far above the charge-ordering transition in $La_{1.67}Sr_{0.33}NiO_4$". In: *Phys. Rev. Lett.* 111 (2013), p. 096404. DOI: 10.1103/PhysRevLett.111.096404. URL: http://link.aps.org/doi/10.1103/PhysRevLett.111.096404

132. **Billinge, S. J. L.** "Pair distribution function technique: principles and methods". In: *Uniting Electron Crystallography and Powder Diffraction*. Ed. by U. Kolb, W. I. F. David, and K. Shankland. NATO Science for Peace and Security Series B: Physics and Biophysics. Dordrecht: Springer Science & Business Media, 2013. Chap. 17, pp. 179 –190. DOI: 10.1007/978-94-007-5580-2. URL: http://doi.org/10.1007/978-94-007-5580-2

133. **Billinge, Simon J. L.** and Christopher L. Farrow. "Towards a robust *ad-hoc* data correction approach that yields reliable atomic pair distribution functions from powder diffraction data". In: *J. Phys: Condens. Mat.* 25 (2013), p. 454202. DOI: 10.1088/0953-8984/25/45/454202. URL: http://doi.org/10.1088/0953-8984/25/45/454202

134. **Billinge, Simon J. L.** "Nanoparticle structures served up on a tray". In: *Nature* 495 (2013), pp. 453–454. URL: http://www.nature.com/nature/journal/v495/n7442/full/495453a.html

135. Emil S. Božin, Pavol Juhás, and **Billinge, Simon J. L.** "Local structure of bulk and nanocrystalline semiconductors using total scattering methods". In: *Characterization of semiconductor heterostructures and nanostructures*. Ed. by Giovanni Agostini and Carlo Lamberti. 2nd. Amsterdam: Elsevier, 2013, pp. 229–257

136. Timur Davis, Matthew Johnson, and **Billinge, Simon J. L.** "Towards phase quantification at the nanoscale using the total scattering pair distribution function (TSPDF) method: recrystallization of cryomilled sulfamerazine". In: *Cryst. Growth Des.* 13 (2013), 4239–4244. URL: http://pubs.acs.org/doi/abs/10.1021/cg400179p

137. Christopher L. Farrow, D. Kwabena Bediako, Yogesh Surendranath, Daniel G. Nocera, and **Billinge, Simon J. L.** "Intermediate-range structure of self-assembled cobalt-based oxygen evolving catalysts". In: *J. Am. Chem. Soc.* 135 (2013), pp. 6403–6406. DOI: 10.1021/ja401276f. URL: http://dx.doi.org/10.1021/ja401276f

138. Simon D. M. Jacques, Marco Di Michiel, Simon A. J. Kimber, Xiaohao Yang, Robert J. Cernik, Andrew M. Beale, and **Billinge, Simon J. L.** "Pair distribution function computed tomography". In: *Nat. Commun.* 4 (2013), p. 2536. DOI: 10.1038/ncomms3536. URL: http://www.nature.com/ncomms/2013/130930/ncomms3536/full/ncomms3536.html

139. P. Juhás, T. Davis, C. L. Farrow, and **Billinge, S. J. L.** "PDFgetX3: A rapid and highly automatable program for processing powder diffraction data into total scattering pair distribution functions". In: *J. Appl. Crystallogr.* 46 (2013), pp. 560–566. DOI: 10.1107/S0021889813005190. URL: http://dx.doi.org/10.1107/S0021889813005190

140. Chenyang Shi, Erin L. Redmond, Amir Mazaheripour, Pavol Juhás, Thomas F. Fuller, and **Billinge, Simon J. L.** "Evidence for anomalous bond softening and disorder below 2 nm diameter in carbon supported platinum nanoparticles from the temperature dependent peak width of the atomic pair distribution function". In: *J. Phys. Chem. C* 117 (2013), pp. 7226–7230. DOI: 10.1021/jp402591s. URL: http://pubs.acs.org/doi/abs/10.1021/jp402591s

141. P. Tian, W. Zhou, J. Liu, Y. Shang, C. L. Farrow, P. Juhás, and **Billinge, S. J. L.** "SrRietveld: A program for automating Rietveld refinements for high throughput studies". In: *J. Appl. Crystallogr.* 46 (2013), pp. 255–258. DOI: 10.1107/S0021889812045967. URL: http://dx.doi.org/10.1107/S0021889812045967

142. Xiaohao Yang, Ahmad S. Masadeh, James R. McBride, Emil S. Božin, Sandra J. Rosenthal, and **Billinge, Simon J. L.** "Confirmation of disordered structure of ultrasmall CdSe nanoparticles from x-ray atomic pair distribution function analysis". In: *Phys. Chem. Chem. Phys.* 15.22 (2013), pp. 8480–8486. DOI: 10.1039/C3CP00111C. URL: http://pubs.rsc.org/en/content/articlelanding/2013/cp/c3cp00111c

143. Milinda Abeykoon, Christos D. Malliakas, Pavol Juhás, Emil S. Božin, Mercouri G. Kanatzidis, and **Billinge, Simon J. L.** "Quantitative nanostructure characterization using atomic pair distribution functions obtained from laboratory electron microscopes". In: *Z. Kristallogr.* 227.5 (2012). Highlighted on the journal cover, pp. 248–256. DOI: 10.1524/zkri.2012.1510. URL: http://www.degruyter.com/view/j/zkri.2012.227.issue-5/zkri.2012.1510/zkri.2012.1510.xml

144. **Billinge, S. J. L.**, P. Juhás, and E. S. Božin. "Fundamentals of pair distribution function analysis". In: *Crystallography for Health and Biosciences*. Ed. by A. Guagliardi and Norberto Masciocchi. Insubria, Como, Italy: Insubria University Press, 2012, pp. 163–176

145. Emil S. Božin, T. Chatterji, and **Billinge, Simon J. L.** "Local structure of ReO_3 at ambient pressure from neutron total scattering study". In: *Phys. Rev. B* 86 (2012), p. 094110. DOI: 10.1103/PhysRevB.86.094110. URL: http://link.aps.org/doi/10.1103/PhysRevB.86.094110

146. T. Egami and **Billinge, S. J. L.** *Underneath the Bragg peaks: structural analysis of complex materials*. 2nd. Amsterdam: Elsevier, 2012. URL: http://store.elsevier.com/product.jsp?lid=0\&iid=73\&sid=0\&isbn=9780080971414

147. Kirsten M. Ø Jensen, Mogens Christensen, Pavol Juhás, Christoffer Tyrsted, Espen D. Bøjesen, Nina Lock, **Billinge, Simon J. L.**, and Bo B. Iversen. "Revealing the mechanisms behind SnO_2 nanoparticle formation and growth during hydrothermal synthesis: an in situ total scattering study". In: *J. Am. Chem. Soc.* 134 (2012), pp. 6785 –6792. DOI: 10.1021/ja300978f. URL: http://dx.doi.org/10.1021/ja300978f

148. Kirsten M. Ø. Jensen, Emil S. Božin, Christos D. Malliakas, Matthew B. Stone, Mark D. Lumsden, Mercouri G. Kanatzidis, Stephen M. Shapiro, and **Billinge, Simon J. L.** "Lattice dynamics reveals a local symmetry breaking in the emergent dipole phase of PbTe". In: *Phys. Rev. B* 86 (2012). Selected as PRB Editor's Suggestion paper, p. 085313. DOI: 10.1103/PhysRevB.86.085313. URL: http://prb.aps.org/abstract/PRB/v86/i8/e085313

149. Erin L. Redmond, Brian P. Setzler, Pavol Juhás, **Billinge, Simon J. L.**, and Thomas F. Fuller. "In-situ monitoring of particle growth at PEMFC cathode under accelerated cycling conditions". In: *Electrochem. Solid St.* 15.5 (2012), B72–B74. DOI: 10.1149/2.004206esl. URL: http://dx.doi.org/10.1149/2.004206esl

150. Christoffer Tyrsted, Kirsten Marie Ørnsbjerg Jensen, Espen Drath Bøjesen, Nina Lock, Mogens Christensen, **Billinge, Simon J. L.**, and Bo Brummerstedt Iversen. "Understanding the formation and evolution of ceria nanoparticles under hydrothermal conditions". In: *Angew. Chem. Int. Edit.* 51 (2012). Selected by the editors as a "Hot" paper for highlighting, pp. 9030–9033. DOI: 10.1002/anie.201204747. URL: http://onlinelibrary.wiley.com/doi/10.1002/anie.201204747/suppinfo

151. Mengqiang Zhu, Christopher L. Farrow, Jeffrey E. Post, Kenneth J. T. Livi, **Billinge, Simon J. L.**, Matthew Ginder-Vogel, and Donald L. Sparks. "Structural study of biotic and abiotic poorly-crystalline manganese oxides using atomic pair distribution function analysis". In: *Geochim. Cosmochim. Ac.* 81 (2012), pp. 39–55. DOI: 10.1016/j.gca.2011.12.006. URL: http://www.sciencedirect.com/science/article/pii/S0016703711007277

152. **Billinge, Simon J. L.** "Hard x-ray lasers take their first steps towards nanostructure solution". In: *Condensed Matter Physics Journal Club* (2011). URL: http://www.condmatjournalclub.org/?p=1392

153. C. H. Booth, E. D. Bauer, Božin E. S., **Billinge, S. J. L.**, and M. D. Walter. "Pair-distribution function analysis of the structural valence transition in $Cp_2^*Yb(4,4'\text{-}Me_2\text{-bipy})$". In: *J. Phys.: Conf. Ser.* 273 (2011), p. 012149. URL: http://iopscience.iop.org/article/10.1088/1742-6596/273/1/012149/meta

154. E. S. Božin, A. S. Masadeh, Y. S. Hor, J. F. Mitchell, and **Billinge, S. J. L.** "Detailed mapping of the local Ir^{4+} dimers through the metal-insulator transitions of $CuIr_2S_4$ thiospinel by x-ray atomic pair distribution function measurements". In: *Phys. Rev. Lett.* 106 (2011), p. 045501. DOI: 10.1103/PhysRevLett.106.045501. URL: http://prl.aps.org/abstract/PRL/v106/i4/e045501

155. Brandi M. Cossairt, Pavol Juhás, **Billinge, Simon J. L.**, and Jonathan S. Owen. "Tuning the surface structure and optical properties of CdSe clusters using coordination chemistry". In: *J. Phys. Chem. Lett.* 2 (2011), pp. 3075–3080. DOI: 10.1021/jz2013769. URL: http://pubs.acs.org/doi/abs/10.1021/jz2013769

156. Timur Dykhne, Ryan Taylor, Alastair Florence, and **Billinge, Simon J. L.** "Data requirements for the reliable use of atomic pair distribution functions in amorphous pharmaceutical fingerprinting". In: *Pharmaceut. Res.* 28 (2011), pp. 1041–1048. DOI: 10.1007/s11095-010-0350-0. URL: http://link.springer.com/article/10.1007/s11095-010-0350-0

157. Christopher L. Farrow, Margaret Shaw, Hyun-Jeong Kim, Pavol Juhás, and **Billinge, Simon J. L.** "The Nyquist-Shannon sampling theorem and the atomic pair distribution function". In: *Phys. Rev. B* 84 (2011), p. 134105. DOI: 10.1103/PhysRevB.84.134105. URL: http://link.aps.org/doi/10.1103/PhysRevB.84.134105

158. Rongwei Hu, Hechang Lei, Milinda Abeykoon, Emil S. Bozin, **Billinge, Simon J. L.**, J. B. Warren, Theo Siegrist, and C. Petrovic. "Synthesis, crystal structure, and magnetism of beta-$Fe_{1.00(2)}Se_{1.00(3)}$ single crystals". In: *Phys. Rev. B* 83 (2011), p. 224502. DOI: 10.1103/PhysRevB.83.224502. URL: http://prb.aps.org/abstract/PRB/v83/i22/e224502

159. Shu Li, Peng Tian, Michael Steigerwald, Louis Brus, **Billinge, Simon J. L.**, Paul Zimmerman, and Nicholas Turro. "$HfO_x(OSiEt_3)_{4-2x}$: a highly soluble hafnia nanosponge". In: *Chem. Mater.* (2011). submitted

160. Lorenzo Malavasi, Gianluca A. Artioli, Hyunjeong Kim, Beatrice Maroni, Boby Joseph, Yang Ren, Thomas Proffen, and **Billinge, Simon J. L.** "Local structural investigation of $SmFeAsO_{1-x}F_x$ high temperature superconductors". In: *J. Phys: Condens. Mat.* 23 (2011), p. 272201. DOI: 10.1088/0953-8984/23/27/272201. URL: http://stacks.iop.org/0953-8984/23/i=27/a=272201

161. Erin L. Redmond, Brian P. Setzler, Amir Masaheripour, Pavol Juhás, **Billinge, Simon J. L.**, and Thomas F. Fuller. "Surface energy of supported platinum nanoparticles". In: *ACS Nano.* (2011). submitted

162. William Schmidt, George Leroi, **Billinge, Simon**, Leon Lederman, Audrey Champagne, Richard Hake, Paula Heron, Lillian McDermott, Fred Myers, Roland Otto, Jay Pasachoff, Carl Pennypacker, and Paul Williams. *Towards coherence in science instruction: A framework for science literacy.* Michigan State University Research Report. 2011

163. Peng Tian, Yanhua Zhang, Keerthi Senevirathne, Stephanie L. Brock, Ambesh Dixit, Gavin Lawes, and **Billinge, Simon J. L.** "Diverse structural and magnetic properties of differently prepared MnAs nanoparticles". In: *ACS Nano.* 5 (2011), pp. 2970–2978. DOI: 10.1021/nn200020r. URL: http://pubs.acs.org/doi/abs/10.1021/nn200020r

164. Peng Tian and **Billinge, Simon J. L.** "Testing different methods for estimating uncertainties on Rietveld refined parameters using SrRietveld". In: *Z. Kristallogr.* 226 (2011), pp. 898–904. DOI: 10.1524/zkri.2011.1421. URL: https://www.degruyter.com/view/j/zkri.2011.226.issue-12/zkri.2011.1421/zkri.2011.1421.xml

165. P. Juhás, L. Granlund, S. R. Gujarathi, P. M. Duxbury, and **Billinge, S. J. L.** "Crystal structure solution from experimentally determined atomic pair distribution functions". In: *J. Appl. Crystallogr.* 42.3 (2010), pp. 623–629. DOI: 10.1107/S002188981000988X. URL: http://dx.doi.org/10.1107/S002188981000988X

166. **Billinge, S. J. L.** and E. S. Božin. "Pair distribution function technique: principles and methods". In: *Diffraction at the Nanoscale: Nanocrystals, Defective and Amorphous Materials.* Ed. by Masciocchi Norberto Guagliardi A. Insubria, Como, Italy: Insubria University Press, 2010, pp. 97–106

167. **Billinge, Simon J. L.**, Timur Dykhne, Pavol Juhás, Emil Božin, Ryan Taylor, Alastair J. Florence, and Kenneth Shankland. "Characterisation of amorphous and nanocrystalline molecular materials by total scattering". In: *CrystEngComm* 12.5 (2010), pp. 1366–1368. DOI: 10.1039/b915453a. URL: http://pubs.rsc.org/en/Content/ArticleLanding/2010/CE/b915453a

168. **Billinge, Simon J. L.** "Nanostructure in technicolor". In: *Condensed Matter Physics Journal Club* (2010). URL: http://www.condmatjournalclub.org/?p=963

169. **Billinge, Simon J. L.** "The nanostructure problem". In: *Physics* 3 (2010), p. 25. DOI: 10.1103/Physics.3.25. URL: http://doi.org/10.1103/Physics.3.25

170. V. A. Blagojevic, J. P. Carlo, L. E. Brus, M. L. Steigerwald, Y. J. Uemura, **Billinge, S. J. L.**, W. Zhou, P. Stephens, A. A. Aczel, and G. M. Luke. "Magnetic phase transition in V_2O_3 nanocrystals". In: *Phys. Rev. B* 82 (2010), p. 094453. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.82.094453

171. E. S. Božin, P. Juhás, W. Zhou, M. B. Stone, D. L. Abernathy, A. Huq, and **Billinge, S. J. L.** "Quantitative structure refinement from the ARCS chopper spectrometer". In: *J. Phys.: Conf. Ser.* 251 (2010), p. 012080. DOI: 10.1088/1742-6596/251/1/012080. URL: http://iopscience.iop.org/1742-6596/251/1/012080

172. Emil S. Božin, Christos D. Malliakas, Petros Souvatzis, Thomas Proffen, Nicola A. Spaldin, Mercouri G. Kanatzidis, and **Billinge, Simon J. L.** "Entropically stabilized local dipole formation in lead chalcogenides". In: *Science* 330 (2010), p. 1660. DOI: 10.1126/science.1192759. URL: http://www.sciencemag.org/content/330/6011/1660

173. Paul Evans and **Billinge, Simon J. L.** "Advances in scattering probes for materials". In: *Bulletin of the Materials Research Society* (2010). URL: https://www.cambridge.org/core/journals/mrs-bulletin/article/advances-in-scattering-probes-for-materials/1E28068FF673FA73AA77F633018A4B69

174. C. L. Farrow, C. Y. Ruan, and **Billinge, S. J. L.** "Quantitative nanoparticle structures from electron crystallography data". In: *Phys. Rev. B* 81 (2010), p. 124104. DOI: 10.1103/PhysRevB.81.134104. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.81.134104

175. Carrie A. Simpson, Christopher L. Farrow, Peng Tian, **Billinge, Simon J. L.**, Brian J. Huffman, Kellen M. Harkness, and David E. Cliffel. "Tiopronin gold nanoparticle precursor forms auriophilic ring tetramer". In: *Inorg. Chem.* 49.23 (2010), pp. 10858 –10866. DOI: 10.1021/ic101146e. URL: http://pubs.acs.org/doi/abs/10.1021/ic101146e

176. J. C. Zheng, A. I. Frenkel, L. Wu, J. Hanson, W. Ku, E. S. Božin, **Billinge, S. J. L.**, and Y. Zhu. "Nanoscale disorder and local electronic properties of $CaCu_3Ti_4O_{12}$: An integrated study of electron, neutron and x-ray diffraction, x-ray absorption fine structure and first principles calculations". In: *Phys. Rev. B* 81 (2010), p. 144203. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.81.144203

177. **Billinge, Simon J. L.** "X-ray Specs: 3D nano-scale resolution imaging with x-rays". In: *Condensed Matter Physics Journal Club* (2009). URL: http://www.condmatjournalclub.org/?p=663

178. **Billinge, Simon**, Greg Smith, Al Ekkebus, and Bruce Gaulin. "International Conference on Neutron Scattering 2009 (ICNS09)". In: *Neutron News* 20.4 (2009). DOI: 10.1080/10448630903240730. URL: http://doi.org/10.1080/10448630903240730

179. **Billinge, S. J. L.** "How do your crystals grow?" In: *Nat. Phys.* 5 (2009). [News and Views article, describing Chung, S.-Y., Kim, Y.-M., Kim, J.-G. and Kim, Y.-J. *Nature Phys.* **5**, 68-73 (2009)], pp. 13 –14. DOI: 10.1038/nphys1172. URL: http://doi.org/10.1038/nphys1172

180. E. S. Božin, P. Juhás, W. Zhou, M. B. Stone, D. L. Abernathy, A. Huq, and **Billinge, S. J. L.** "Atomic pair distribution function analysis from the ARCS chopper spectrometer at the Spallation Neutron Source". In: *J. Appl. Crystallogr.* 42 (2009), pp. 724–725. URL: http://scripts.iucr.org/cgi-bin/paper?wf5045

181. C. L. Farrow and **Billinge, S. J. L.** "Relationship between the atomic pair distribution function and small angle scattering: implications for modeling of nanoparticles". In: *Acta Crystallogr. A* 65.3 (2009), pp. 232–239. DOI: 10.1107/S0108767309009714. URL: http://scripts.iucr.org/cgi-bin/paper?cn5017

182. J. E. Greedan, Delphine Gout, A. D. Lozano, Shahab Derahkshan, Th. Proffen, H-J. Kim, E. S. Božin, and **Billinge, S. J. L.** "The Local and average structures of the spin-glass pyrochlore, $Y_2Mo_2O_7$, from neutron diffraction and neutron pair distribution function analysis". In: *Phys. Rev. B* 79 (2009). (highlighted as an "editors' selection"), p. 014427. DOI: 10.1103/PhysRevB.79.014427. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.79.014427

183. H. Lin, E. S. Božin, **Billinge, S. J. L.**, J. Androulakis, C. H. Lin, and M. G. Kanatzidis. "Phase separation and nanostructuring in the thermoelectric material $PbTe_{1-x}S_x$ studied using the atomic pair distribution function technique". In: *Phys. Rev. B* 80 (2009), p. 045204. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.80.045204

184. A. F. Gualtieri, S. Ferrari, M. Leoni, G. Grathoff, R. Hugo, M. Shatnawi, G. Paglia, and **Billinge, S.** "Structural characterization of the clay mineral illite-1M". in: *J. Appl. Crystallogr.* 41.2 (2008), pp. 402–415. DOI: 10.1107/S0021889808004202. URL: http://dx.doi.org/10.1107/S0021889808004202

185. **Billinge, S. J. L.** "Local structure from total scattering and atomic pair distribution function (PDF) analysis". In: *Powder diffraction: theory and practice*. Ed. by Robert E. Dinnebier and Simon J. L. Billinge. Cambridge, UK: Royal Society of Chemistry, 2008. Chap. 16, pp. 464 –493. DOI: 10.1039/9781847558237. URL: http://doi.org/10.1039/9781847558237

186. **Billinge, Simon J. L.** "Nanoparticle structure: going beyond pictures". In: *Condensed Matter Physics Journal Club* (2008). URL: http://www.condmatjournalclub.org/?p=543

187. **Billinge, Simon J. L.** "Towards a Humpty Dumpty approach for solving the structure of individual nanoparticles". In: *Condensed Matter Physics Journal Club* (2008). URL: http://www.condmatjournalclub.org/?p=591

188. **Billinge, Simon J. L.** "Nanoscale structural order from the atomic pair distribution function (PDF): There's plenty of room in the middle". In: *J. Solid State Chem.* 181 (2008), pp. 1695–1700. DOI: 10.1016/j.jssc.2008.06.046. URL: http://doi.org/10.1016/j.jssc.2008.06.046

189. E. S. Božin, A. Sartbaeva, H. Zheng, S. A. Wells, J. F. Mitchell, Th. Proffen, M. F. Thorpe, and **Billinge, S. J. L.** "Structure of $CaMnO_3$ in the range $\mathbf{10K \leq T \leq 550K}$ from neutron time-of-flight total scattering". In: *J. Phys. Chem. Solids* 69 (2008), pp. 2146 –2150. DOI: 10.1016/j.jpcs.2008.03.029. URL: http://www.sciencedirect.com/science/article/pii/S0022369708000917

190. Monica Dapiaggi, HyunJeong Kim, Emil S. Božin, **Billinge, Simon J. L.**, and Gilberto Artioli. "Study of the negative thermal expansion of cuprite-type structures by means of temperature-dependent pair distribution function analysis: Preliminary results". In: *J. Phys. Chem. Solids* 69 (2008), pp. 2182 –2186. DOI: 10.1016/j.jpcs.2008.03.030. URL: http://www.sciencedirect.com/science/article/pii/S0022369708000991

191. P. Juhás, L. Granlund, P. M. Duxbury, W. F. Punch, and **Billinge, S. J. L.** "The Liga algorithm for ab initio determination of nanostructure". In: *Acta Crystallogr. A* 64.6 (2008), pp. 631–640. DOI: 10.1107/S0108767308027591. URL: http://dx.doi.org/10.1107/S0108767308027591

192. Moneeb T. M. Shatnawi, Christopher L. Farrow, Ping Chen, Punit Boolchand, Asel Sartbaeva, M. F. Thorpe, and **Billinge, Simon J. L.** "Search for a structural response to the intermediate phase in Ge_xSe_{1-x} glasses". In: *Phys. Rev. B* 77 (2008), p. 94134. DOI: 10.1103/PhysRevB.77.094134. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.77.094134

193. R. J. Worhatch, H. J. Kim, I. P. Swainson, A. L. Yonkeu, and **Billinge, S. J. L.** "Study of local structure in selected cubic organic-inorganic perovskites". In: *Chem. Mater.* 20 (2008), pp. 1272–1277. URL: http://pubs.acs.org/doi/abs/10.1021/cm702668d

194. **Billinge, Simon J. L.** "Structure solution of real materials: charge flipping can help". In: *Condensed Matter Physics Journal Club* (2007). URL: http://www.condmatjournalclub.org/?p=496

195. **Billinge, S. J. L.** and I. Levin. "The problem with determining atomic structure at the nanoscale". In: *Science* 316 (2007), pp. 561–565. DOI: 10.1126/science.1135080. URL: http://www.sciencemag.org/content/316/5824/561.abstract

196. **Billinge, S. J. L.** "Nanostructure studied using the atomic pair distribution function". In: *Z. Kristallogr. Suppl.* 26 (2007), pp. 17–26. URL: https://www.researchgate.net/publication/237496696_Nanostructure_studied_using_the_atomic_pair_distribution_function

197. E. S. Božin, M. Schmidt, A. J. DeConinck, G. Paglia, J. F. Mitchell, T. Chatterji, P. G. Radaelli, Th. Proffen, and **Billinge, S. J. L.** "Understanding the insulating phase in CMR manganites: Shortening of the Jahn-Teller long-bond across the phase diagram of $La_{1-x}Ca_xMnO_3$". In: *Phys. Rev. Lett.* 98 (2007), p. 137203. DOI: 10.1103/PhysRevLett.98.137203. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.98.137203

198. E. S. Božin, X. Qiu, R. J. Worhatch, G. Paglia, M. Schmidt, P. G. Radaelli, J. F. Mitchell, T. Chatterji, Th. Proffen, and **Billinge, S. J. L.** "Utilizing total scattering to study the Jahn-Teller transition in $La_{1-x}Ca_xMnO_3$". In: *Z. Kristallogr. Suppl.* 26 (2007), pp. 429–434. URL: https://www.researchgate.net/publication/237221028_Utilizing_total_scattering_to_study_the_Jahn-Teller_transition_in_La_1-x_Ca_x_MnO_3

199. G. Campi, Th. Proffen, X. Qiu, E. S. Božin, **Billinge, S. J. L.**, S. Agrestini, N. L. Saini, and A. Bianconi. "Local lattice dynamics in the $Mg_{0.5}Al_{0.5}B_2$ superconductor". In: *J. Supercond. Novel Magn.* 20 (2007), pp. 505–510. DOI: 10.1007/s10948-007-0277-9. URL: http://link.springer.com/article/10.1007/s10948-007-0277-9

200. Shahab Derakhshan, Abdeljalil Assoud, Katja M. Kleinke, Trupti Khaire, Ahmad S. Masadeh, **Billinge, Simon J. L.**, and Holger Kleinke. "Square net distortion engineering in the ternary variants of titanium antimonide, $Ti_{2-\delta}M_\delta Sb$ (M=Zr, Hf)". In: *Intermetallics* 15 (2007), pp. 1071–1077. URL: http://www.sciencedirect.com/science/article/pii/S0966979507000052

201. C. L. Farrow, P. Juhás, Jiwu Liu, D. Bryndin, E. S. Božin, J. Bloch, Th. Proffen, and **Billinge, S. J. L.** "PDFfit2 and PDFgui: Computer programs for studying nanostructure in crystals". In: *J. Phys: Condens. Mat.* 19 (2007), p. 335219. DOI: 10.1088/0953-8984/19/33/335219. URL: http://iopscience.iop.org/0953-8984/19/33/335219/

202. F. Inam, Moneeb T. Shatnawi, D. Tafen, **Billinge, S. J. L.**, P. Chen, and D. A. Drabold. "An intermediate phase in Ge_xSe_{1-x} glasses: experiment and simulation". In: *J. Phys: Condens. Mat.* 19 (2007), p. 455206. DOI: 10.1088/0953-8984/19/45/455206. URL: http://iopscience.iop.org/article/10.1088/0953-8984/19/45/455206/meta

203. H. J. Kim, E. S. Božin, S. M. Haile, G. J. Snyder, and **Billinge, S. J. L.** "Presence of nano-scale α-structural domains in the phonon-glass thermoelectric material β-Zn_4Sb_3". In: *Phys. Rev. B* 75 (2007), p. 134103. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.75.134103

204. Valentin A. Levashov, **Billinge, S. J. L.**, and M. F. Thorpe. "Quantum correction to the pair distribution function". In: *J. Comput. Chem.* 28 (2007), pp. 1865–1882. DOI: 10.1002/jcc.20713. URL: http://onlinelibrary.wiley.com/doi/10.1002/jcc.20713/full

205. L. Malavasi, **Billinge, S. J. L.**, H. J. Kim, Th. Proffen, C. Tealdi, and G. Flor. "Nature of the monoclinic to cubic phase transition in the fast oxygen ion conductor $La_2Mo_2O_9$ (LAMOX)". in: *J. Am. Chem. Soc.* 129 (2007), pp. 6903–6907. URL: http://pubs.acs.org/doi/abs/10.1021/ja071281e

206. A. S. Masadeh, E. S. Božin, C. L. Farrow, G. Paglia, P. Juhás, A. Karkamkar, M. G. Kanatzidis, and **Billinge, S. J. L.** "Quantitative size-dependent structure and strain determination of CdSe nanoparticles using atomic pair distribution function analysis". In: *Phys. Rev. B* 76 (2007), p. 115413. DOI: 10.1103/PhysRevB.76.115413. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.76.115413

207. A. Sartbaeva, S. A. Wells, M. F. Thorpe, E. S. Božin, and **Billinge, S. J. L.** "Quadrupolar Ordering in $LaMnO_3$ Revealed from Scattering Data and Geometric Modeling". In: *Phys. Rev. Lett.* 99 (2007), p. 155503. DOI: 10.1103/PhysRevLett.99.155503. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.99.155503

208. Mouath Shatnawi, Gianluca Paglia, James L. Dye, Kevin D. Cram, Michael Lefenfeld, and **Billinge, Simon J. L.** "Structures of alkali metals in silica gel nanopores: new materials for chemical reductions and hydrogen production". In: *J. Am. Chem. Soc.* 129 (2007), pp. 1386–1392. DOI: 10.1021/ja067140e. URL: http://dx.doi.org/10.1021/ja067140e

209. Hasan Yavas, E. Ercan Alp, Harald Sinn, Ahmet Alatas, Ayman Said, Yuri Shvyd'ko, Thomas Toellner, Ruben Khachatryan, **Billinge, Simon J. L.**, M. Zahid Hasan, and Wolfgang Sturhahn. "Sapphire analyzers for high-resolution x-ray spectroscopy". In: *Nucl. Instrum. Methods A* 582 (2007), pp. 149–151. DOI: 10.1016/j.nima.2007.08.095. URL: http://www.sciencedirect.com/science/article/pii/S0168900207017834#

210. **Billinge, S. J. L.** "Structure Determination and Phase Analysis using Neutron Diffraction". In: *JOM-J. Min. Met. Mat. S.* 58 (2006), pp. 47–51. URL: http://www.tms.org/pubs/journals/JOM/0603/Billinge-0603.html

211. **Billinge, S. J. L.**, K. Rajan, and S. B. Sinnott. "From Cyberinfrastructure to Cyberdiscovery in Materials Science: Enhancing outcomes in materials research, education and outreach". Report of the NSF-DMR Cyberinfrastructure Steering Committee, 2006. http://www.mcc.uiuc.edu/nsf/ciw_2006/. 2006. URL: http://www.mcc.uiuc.edu/nsf/ciw_2006/

212. E. S. Božin, X. Qiu, M. Schmidt, G. Paglia, J. F. Mitchell, P. G. Radaelli, Th. Proffen, and **Billinge, S. J. L.** "Local structural aspects of the orthorhombic to pseudo-cubic phase transformation in $La_{1-x}Ca_xMnO_3$". In: *Physica B* 385-386 (2006), pp. 110–112. URL: http://www.sciencedirect.com/science/article/pii/S0921452606010143

213. G. Campi, E. Cappelluti, Th. Proffen, X. Qiu, E. S. Božin, **Billinge, S. J. L.**, S. Agrestini, N. L. Saini, and A. Bianconi. "Study of temperature dependent atomic correlations in MgB_2". In: *Eur. Phys. J. B* 52 (2006), pp. 15–21. DOI: 10.1140/epjb/e2006-00269-7. URL: http://link.springer.com/article/10.1140/epjb/e2006-00269-7

214. P. Juhás, D. M. Cherba, P. M. Duxbury, W. F. Punch, and **Billinge, S. J. L.** "Ab initio determination of solid-state nanostructure". In: *Nature* 440.7084 (2006), pp. 655–658. DOI: 10.1038/nature04556. URL: http://www.nature.com/nature/journal/v440/n7084/abs/nature04556.html

215. H. J. Kim, C. D. Malliakas, A. Tomic, S. H. Tessmer, M. G. Kanatzidis, and **Billinge, S. J. L.** "Local atomic structure and discommensurations in the charge density wave of $CeTe_3$". In: *Phys. Rev. Lett.* 96 (2006), p. 226401. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.96.226401

216. G. Paglia, E. S. Božin, D. Vengust, D. Mihailovic, and **Billinge, S. J. L.** "Accurate structure determination of $Mo_6S_yI_z$ nanowires from PDF analysis". In: *Chem. Mater.* 18 (2006), pp. 100–106. DOI: 10.1021/cm051833x. URL: http://dx.doi.org/10.1021/cm051833x

217. G. Paglia, E. S. Božin, and **Billinge, S. J. L.** "Fine-Scale Nanostructure in γ-Al_2O_3". In: *Chem. Mater.* 18.14 (2006), pp. 3242–3248. DOI: 10.1021/cm060277j. URL: http://dx.doi.org/10.1021/cm060277j

218. A. Sartbaeva, S. A. Wells, M. F. Thorpe, E. S. Bozin, and **Billinge, S. J. L.** "Geometric Simulation of Perovskite Frameworks with Jahn-Teller Distortions: Applications to the Cubic Manganites". In: *Phys. Rev. Lett.* 97 (2006), p. 065501. DOI: 10.1103/PhysRevLett.97.065501. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.97.065501

219. **Billinge, Simon J. L.**, Emily J. McKimmey, Mouath Shatnawi, Hyun Jeong Kim, Valeri Petkov, Didier Wermeille, and Thomas J. Pinnavaia. "Mercury Binding Sites in Thiol-Functionalized Mesostructured Silica". In: *J. Am. Chem. Soc.* 127 (2005), pp. 8492–8498. DOI: 10.1021/ja0506859. URL: http://doi.org/10.1021/ja0506859

220. E. S. Božin and **Billinge, S. J. L.** "Nominal doping and partition of doped holes between planar and apical orbitals in $La_{2-x}Sr_xCuO_4$". In: *Phys. Rev. B* 72 (2005), p. 174427. URL: http://link.aps.org/abstract/PRB/v72/e174427

221. S. Brühne, E. Uhrig, C. Gross, W. Assmus, A. S. Masadeh, and **Billinge, S. J. L.** "The local atomic quasicrystal structure of the icosahedral $Mg_{25}Y_{11}Zn_{64}$ alloy". In: *J. Phys: Condens. Mat.* 17 (2005), pp. 1561–1572. URL: http://iopscience.iop.org/article/10.1088/0953-8984/17/10/011/meta

222. S. Brühne, E. Uhrig, K. D. Luther, W. Assmus, M. Brunelli, A. S. Masadeh, and **Billinge, S. J. L.** "PDF from X-ray powder diffraction for nanometer-scale atomic structure analysis of quasicrystalline alloys". In: *Z. Kristallogr.* 220 (2005), pp. 962–967. URL: https://www.degruyter.com/view/j/zkri.2005.220.issue-11/zkri.2005.220.11_2005.962/zkri.2005.220.11_2005.962.xml

223. David Cherba, William Punch, Phil Duxbury, **Billinge, Simon J. L.**, and Pavol Juhás. "Conformation of an Ideal Bucky Ball Molecule by Genetic Algorithm and Geometric Constraint from Pair Distance Data". In: *GECCO-2005, Genetic and Evolutionary Computation Conference Proceedings*. New York, 2005. URL: http://dl.acm.org/citation.cfm?id=1068261

224. V. A. Levashov, **Billinge, S. J. L.**, and M. F. Thorpe. "Density fluctuations and the pair distribution function". In: *Phys. Rev. B* 72 (2005), p. 024111. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.72.024111

225. He Lin, E. S. Božin, **Billinge, S. J. L.**, Eric Quarez, and M. G. Kanatzidis. "Nanoscale clusters in the high performance thermoelectric $AgPb_mSbTe_{m+2}$". In: *Phys. Rev. B* 72 (2005), p. 174113. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.72.174113

226. C. Malliakas, **Billinge, S. J. L.**, H. J. Kim, and M. G. Kanatzidis. "Square nets of tellurium: Rare-earth dependent variation in the charge-density wave of $RETe_3$ (RE= rare earth element)". In: *J. Am. Chem. Soc.* 127 (2005), pp. 6510–6511. URL: http://pubs.acs.org/doi/abs/10.1021/ja0505292

227. Xiangyun Qiu, Th. Proffen, J. F. Mitchell, and **Billinge, S. J. L.** "Orbital correlations in the pseudocubic O and rhombohedral R-phases of $LaMnO_3$". In: *Phys. Rev. Lett.* 94 (2005), p. 177203. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.94.177203

228. S. Vensky, L. Kienle, R. E. Dinnebier, A. S. Masadeh, **Billinge, S. J. L.**, and M. Jansen. "The real structure of Na_3BiO_4 by electron microscopy, HR-XRD and PDF analysis". In: *Z. Kristallogr.* 220 (2005), pp. 231–244. URL: https://www.degruyter.com/view/j/zkri.2005.220.issue-2-3/zkri.220.2.231.59119/zkri.220.2.231.59119.xml

229. **Billinge, S. J. L.** and M. G. Kanatzidis. "Beyond crystallography: the study of disorder, nanocrystallinity and crystallographically challenged materials". In: *Chem. Commun.* 7 (2004), pp. 749–760. DOI: 10.1039/b309577k. URL: http://doi.org/10.1039/b309577k

230. **Billinge, S. J. L.** "The atomic pair distribution function: past and present". In: *Z. Kristallogr.* 219 (2004), pp. 117–121. DOI: 10.1524/zkri.219.3.117.29094. URL: http://doi.org/10.1524/zkri.219.3.117.29094

231. E. S. Božin, V. Petkov, P. W. Barnes, P. M. Woodward, T. Vogt, S. D. Mahanti, and **Billinge, S. J. L.** "Temperature dependent total scattering structural study of $CaCu_3Ti_4O_{12}$". In: *J. Phys: Condens. Mat.* 16 (2004), S5091–S5102. URL: http://iopscience.iop.org/0953-8984/16/44/007

232. P. J. Chupas, S. Chaudhuri, J. C. Hanson, X. Qiu, P. L. Lee, S. D. Shastri, **Billinge, S. J. L.**, and C. P. Grey. "Probing local and long-range structure simultaneously: an in-situ study of the high-temperature phase transition of α-AlF_3". In: *J. Am. Chem. Soc.* 126 (2004), pp. 4756–4757. URL: http://pubs.acs.org/doi/abs/10.1021/ja031553n

233. Shahab Derakhshan, Abdeljalil Assoud, Enkhtsetseg Dashjav, Xiangyun Qiu, **Billinge, Simon J. L.**, and Holger Kleinke. "Planar nets of Ti atoms comprising squares and rhombs in the new binary antimonide Ti_2Sb". In: *J. Am. Chem. Soc.* 126 (26 2004), pp. 8295–8302. URL: http://pubs.acs.org/doi/abs/10.1021/ja048262e

234. Pantelis N. Trikalitis, Nan Ding, Chris Malliakas, **Billinge, Simon J. L.**, and Mercouri G. Kanatzidis. "Mesostructured Selenides with Cubic MCM-48 Type Symmetry: Large Framework Elasticity and Uncommon Resiliency to Strong Acids". In: *J. Am. Chem. Soc.* 126 (2004), pp. 15326–15327. URL: http://pubs.acs.org/doi/abs/10.1021/ja044954r

235. Xiangyun Qiu, Jeroen W. Thompson, and **Billinge, Simon J. L.** "PDFgetX2: a GUI driven program to obtain the pair distribution function from X-ray powder diffraction data". In: *J. Appl. Crystallogr.* 37 (2004), p. 678. URL: http://www.pa.msu.edu/cmp/billinge-group/programs/PDFgetX2

236. Xiangyun Qiu, Emil S. Božin, Pavol Juhás, Thomas Proffen, and **Billinge, Simon J. L.** "Reciprocal space instrumental effects on the real space neutron atomic pair distribution function". In: *J. Appl. Crystallogr.* 37 (2004), pp. 110–116. URL: http://scripts.iucr.org/cgi-bin/paper?ko5004

237. X. Qiu, **Billinge, S. J. L.**, C. R. Kmety, and J. F. Mitchell. "Evidence for nano-scale inhomogeneities in bilayer manganites in the Mn^{4+} rich region: $0.54 \leq x \leq 0.80$". In: *J. Phys. Chem. Solids* 65 (8–9 2004), pp. 1423–1429. URL: http://www.sciencedirect.com/science/article/pii/S0022369704000381

238. M. Schmidt, P. G. Radaelli, M. J. Gutmann, **Billinge, S. J. L.**, N. Hur, and S. W. Cheong. "Temperature-induced barium de-trapping from a double-well potential in Ba_6Ge_{25}". In: *J. Phys: Condens. Mat.* 16 (2004), pp. 7287–7302. URL: http://iopscience.iop.org/article/10.1088/0953-8984/16/41/010/meta

239. B. H. Toby and **Billinge, S. J. L.** "Determination of standard uncertainties in fits to pair distribution functions". In: *Acta Crystallogr. A* 60 (2004), pp. 315–317. URL: http://scripts.iucr.org/cgi-bin/paper?th5001

240. Peter J. Chupas, Clare P. Grey, Jonathan C. Hanson, Jae-Yong Kim, Jose Rodriguez, Xiangyun Qiu, **Billinge, Simon J. L.**, and Peter L. Lee. "In-situ time resolved powder diffraction studies in heterogenous catalysis; coupling the study of long range and local structural changes". In: *Commission on Powder Diffraction Newsletter, International Union of Crystallography* 29 (2003), pp. 24–25

241. **Billinge, S. J. L.** "Strain, nano-phase separation, multi-scale structures and function of advanced materials". In: *Intrinsic Multiscale Structure and Dynamics of Complex Electronic Oxides*. Ed. by S. Shenoy and A. R. Bishop. Singapore: World Scientific, 2003, pp. 25 –40. DOI: 10.1142/9789812705112_0004. URL: http://www.worldscientific.com/doi/abs/10.1142/9789812705112_0004

242. Peter J. Chupas, Xiangyun Qiu, J. C. Hanson, P. L. Lee, Clare P. Grey, and **Billinge, Simon J. L.** "Rapid acquisition pair distribution function analysis (RA-PDF)". in: *J. Appl. Crystallogr.* 36 (2003), pp. 1342–1347. DOI: 10.1107/S0021889803017564. URL: http://scripts.iucr.org/cgi-bin/paper?wf5000

243. T. Egami and **Billinge, S. J. L.** *Underneath the Bragg peaks: structural analysis of complex materials*. Oxford, England: Pergamon Press, Elsevier, 2003

244. **Billinge, S. J. L.**, M. Gutmann, and E. S. Božin. "Structural response to local charge order in underdoped but superconducting $La_{2-x}(Sr,Ba)_xCuO_4$". In: *Int. J. Mod. Phys. B* 17 (2003), p. 3640. DOI: 10.1142/S021797920302154X. URL: http://www.worldscinet.com/ijmpb/17/1718n20/S021797920302154X.html

245. I. K. Jeong, R. H. Heffner, M. J. Graf, and **Billinge, S. J. L.** "Lattice dynamics and correlated atomic motion from the atomic pair distribution function". In: *Phys. Rev. B* 67 (2003), p. 104301. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.67.104301

246. P. F. Peterson, E. S. Božin, Th. Proffen, and **Billinge, S. J. L.** "Improved measures of quality for atomic pair distribution functions". In: *J. Appl. Crystallogr.* 36 (2003), p. 53. DOI: 10.1107/S0021889802018708. URL: http://dx.doi.org/10.1107/S0021889802018708

247. Th. Proffen, **Billinge, S. J. L.**, T. Egami, and D. Louca. "Structural analysis of complex materials using the atomic pair distribution function - a practical guide". In: *Z. Kristallogr.* 218 (2003), pp. 132–143. URL: https://www.degruyter.com/view/j/zkri.2003.218.issue-2/zkri.218.2.132.20664/zkri.218.2.132.20664.xml

248. **Billinge, S. J. L.** and P. M. Duxbury. "Structural compliance, misfit strain and stripe nanostructures in cuprate superconductors; implications and experimental observations". In: *Int. J. Mod. Phys. B* 16 (2002), p. 1697. URL: http://www.worldscientific.com/doi/abs/10.1142/S0217979202011275

249. **Billinge, S. J. L.** and P. M. Duxbury. "Structural compliance, misfit strain and stripe nanostructures in cuprate superconductors". In: *Phys. Rev. B* 66 (2002), p. 064529. DOI: 10.1103/PhysRevB.66.064529. URL: http://dx.doi.org/10.1103/PhysRevB.66.064529

250. **Billinge, S. J. L.** "Complex materials: beyond crystallography". In: *Z. Kristallogr.* 217 (2002). invited contribution, p. 282. DOI: 10.1524/zkri.217.7.282.23674. URL: http://doi.org/10.1524/zkri.217.7.282.23674

251. B. J. Campbell, **Billinge, S. J. L.**, J. W. Lynn, R. Osborn, and S. K. Sinha. "The structure of Jahn-Teller polarons in the colossal magnetoresistive manganites". In: *From semiconductors to proteins: beyond the average structure*. Ed. by S. J. L. Billinge and M. F. Thorpe. New York: Kluwer/Plenum, 2002, p. 183. URL: http://link.springer.com/chapter/10.1007/978-1-4615-0613-3_11#page-1

252. M. G. Gutmann, E. S. Božin, **Billinge, S. J. L.**, N. A. Babushkina, L. M. Belova, A. R. Kaul, and O. Yu Gorbenko. "Temperature evolution of the local atomic structure in oxygen isotope substituted $Pr_{0.525}La_{0.175}Ca_{0.3}MnO_3$". In: *Appl. Phys. A* 74 (2002), p. 892. DOI: 10.1007/s003390201672. URL: http://link.springer.com/article/10.1007%2Fs003390201672

253. T. R. Pauly, V. Petkov, Y. Liu, **Billinge, S. J. L.**, and T. J. Pinnavaia. "Role of framework sodium versus local framework structure in determining the hydrothermal stability of MCM-41 mesostructures". In: *J. Am. Chem. Soc.* 124 (2002), pp. 99–105. URL: http://pubs.acs.org/doi/abs/10.1021/ja0118183

254. V. Petkov and **Billinge, S. J. L.** "From crystals to nanocrystals: semiconductors and beyond". In: *From semiconductors to proteins: beyond the average structure*. Ed. by S. J. L. Billinge and M. F. Thorpe. New York: Kluwer/Plenum, 2002, p. 153. URL: http://link.springer.com/chapter/10.1007/978-1-4615-0613-3_9

255. V. Petkov, P. N. Trikalitis, E. S. Bozin, **Billinge, S. J. L.**, T. Vogt, and M. G. Kanatzidis. "Structure of $V_2O_5.nH_2O$ xerogel solved by the atomic pair distribution function technique". In: *J. Am. Chem. Soc.* 124 (2002), p. 10157. URL: http://pubs.acs.org/doi/abs/10.1021/ja026143y

256. V. Petkov, **Billinge, S. J. L.**, P. Larson, S. D. Mahanti, T. Vogt, K. K. Rangan, and M. G. Kanatzidis. "Structure of nanocrystalline materials using atomic pair distribution function analysis: study of $LiMoS_2$". In: *Phys. Rev. B* 65 (2002), p. 092105. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.65.092105

257. V. Petkov, **Billinge, S. J. L.**, T. Vogt, A. S. Ichimura, and J. L. Dye. "Structure of intercalated Cs in zeolite ITQ-4: an array of metal ions and electrons confined in a pseudo-1D nanoporous host". In: *Phys. Rev. Lett.* 89 (2002). (Highlighted in Phys. Rev. Focus:

http://focus.aps.org/story/v10/st4), p. 075502. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.89.075502

258. Th. Proffen, T. Egami, **Billinge, S. J. L.**, A. K. Cheetham, D. Louca, and J. B. Parise. "Building a high resolution total scattering powder diffractometer - upgrade of NPD at MLNSC". in: *Appl. Phys. A* 74 (2002), s163–s165. URL: http://link.springer.com/article/10.1007/s003390201929

259. Th. Proffen and **Billinge, S. J. L.** "Probing the local structure of doped manganites using the atomic pair distribution function". In: *Appl. Phys. A* 74 (2002), p. 1770. URL: http://link.springer.com/article/10.1007/s003390201846

260. Th. Proffen, V. Petkov, **Billinge, S. J. L.**, and T. Vogt. "Chemical short range order obtained from the atomic pair distribution function". In: *Z. Kristallogr.* 217 (2002), p. 47. URL: https://www.degruyter.com/view/j/zkri.2002.217.issue-2/zkri.217.2.47.20626/zkri.217.2.47.20626.xml

261. D. V. Sheptyakov, A. M. Abakumov, E. V. Antipov, A. M. Balagurov, **Billinge, S. J. L.**, P. Fischer, L. Keller, M. V. Lobanov, B. Ph. Pavlyuk, V. Yu. Pomjakushin, and M. G. Rozova. "Crystal and magnetic structures of new layered oxides A_2GaMnO_{5+y} (A=Ca, Sr)". In: *Appl. Phys. A* 74 (2002), p. 1734. URL: http://link.springer.com/article/10.1007/s003390201842

262. M. F. Thorpe, V. A. Levashov, M. Lei, and **Billinge, S. J. L.** "Notes on the analysis of data for pair distribution functions". In: *From semiconductors to proteins: beyond the average structure*. Ed. by S. J. L. Billinge and M. F. Thorpe. New York: Kluwer/Plenum, 2002, pp. 105–128. URL: http://link.springer.com/chapter/10.1007/978-1-4615-0613-3_7

263. V. Yu. Pomjakushin, A. M. Balagurov, T. V. Elzhov, D. V. Sheptyakov, P. Fischer, D. I. Khomskii, V. Yu. Yushankhai, A. M. Abakumov, M. G. Rozova, E. V. Antipov, M. V. Lobanov, and **Billinge, S. J. L.** "Atomic and magnetic structures, disorder effects and unconventional superexchange interactions in $A_2MnGaO_{5+\delta}$ (A=Sr,Ca) oxides with layered brownmillerite-type structure". In: *Phys. Rev. B* 66 (2002), p. 184412. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.66.184412

264. P. F. Peterson, Th. Proffen, I. -K. Jeong, **Billinge, S. J. L.**, K.-S. Choi, M. G. Kanatzidis, and P. G. Radaelli. "Local atomic strain in $ZnSe_{1-x}Te_x$ from high real space resolution neutron pair distribution function measurements". In: *Phys. Rev. B* 63 (16 2001), p. 165211. DOI: 10.1103/PhysRevB.63.165211. URL: http://link.aps.org/doi/10.1103/PhysRevB.63.165211

265. I. -K. Jeong, J. Thompson, A. M. P. Turner, and **Billinge, S. J. L.** "PDFgetX: a program for determining the atomic pair distribution function from X-ray powder diffraction data". In: *J. Appl. Crystallogr.* 34 (2001), p. 536. DOI: 10.1107/S0021889801009207. URL: http://journals.iucr.org/j/issues/2001/04/00/

266. I. -K. Jeong, F. Mohiuddin-Jacobs, V. Petkov, **Billinge, S. J. L.**, and S. Kycia. "Local structure study of $In_xGa_{1-x}As$ semiconductor alloys using high energy synchrotron X-ray diffraction". In: *Phys. Rev. B* 63 (2001), p. 205202. DOI: 10.1103/PhysRevB.63.205202. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.63.205202

267. R. Patschke, J. D. Breshears, P. Brazis, C. R. Kannewurf, **Billinge, S. J. L.**, and M. G. Kanatzidis. "Cu_xUTe_3: Stabilization of UTe_3 in the $ZrSe_3$ Structure Type via Copper Insertion. The Artifact of Te-Te Chains and Evidence for Distortions Due to Long Range Modulations". In: *J. Am. Chem. Soc.* 123 (2001), p. 4755. DOI: 10.1021/ja0042534. URL: http://pubs.acs.org/doi/abs/10.1021/ja0042534

268. V. Petkov, M. G. Kanatzidis, T. Vogt, and **Billinge, S. J. L.** "Structure of crystallographically challenged materials by profile analysis of atomic pair distribution functions: study of $LiMoS_2$ and mesostructured $MnGe_4S_{10}$". In: *Mater. Res. Soc. Symp. Proc.* 678 (2001), p. 151. URL: https://www.cambridge.org/core/journals/mrs-online-proceedings-library-archive/article/structure-of-crystallographically-challenged-materials-by-profile-analysis-of-atomic-pair-distribution-functions-study-of-limos2-and-mesostructured-mnge4s10/841A90E030E7EE031FDF6E24BE7887B7

269. V. Petkov and **Billinge, S. J. L.** "Local structure of random $In_xGa_{1-x}As$ alloys by full-profile fitting of atomic pair distribution functions". In: *Physica B* 305 (2001), p. 83. URL: http://www.sciencedirect.com/science/article/pii/S0921452601005518

270. Th. Proffen, R. B. Neder, and **Billinge, S. J. L.** "Teaching diffraction using computer simulations over the internet". In: *J. Appl. Crystallogr.* 34 (2001), p. 767. URL: http://scripts.iucr.org/cgi-bin/paper?os0080

271. P. F. Peterson, M Gutmann, Th. Proffen, and **Billinge, S. J. L.** "PDFgetN: a user-friendly program to extract the total scattering structure function and the pair distribution function from neutron powder diffraction data". In: *J. Appl. Crystallogr.* 33.4 (2000), pp. 1192–1192. DOI: 10.1107/S0021889800007123. URL: http://dx.doi.org/10.1107/S0021889800007123

272. **Billinge, S. J. L.**, V. Petkov, and Th. Proffen. "Structure on different length scales from powder diffraction: the real-space pair distribution function (PDF) technique". In: *Commission on Powder Diffraction of the International Union of Crystallography, Newsletter number 24* (2000)

273. **Billinge, S. J. L.**, E. S. Božin, M. Gutmann, and H. Takagi. "Microscopic charge inhomogeneities in underdoped $La_{2-x}Sr_xCuO_4$: local structural evidence". In: *J. Supercond.* 13 (2000), p. 713. URL: http://doi.org/10.1023/A:1007801928742

274. **Billinge, S. J. L.**, M. Gutmann, and E. S. Bozin. "Local structure as a probe of stripes and its relation to T^*". In: *Physica C* 341-348 (2000), p. 1795. DOI: 10.1016/S0921-4534(00)01077-7. URL: http://doi.org/10.1016/S0921-4534(00)01077-7

275. **Billinge, S. J. L.**, Th. Proffen, V. Petkov, J. L. Sarrao, and S. Kycia. "Evidence for charge localization in the ferromagnetic phase of $La_{1-x}Ca_xMnO_3$ from high real-space-resolution X-ray diffraction". In: *Phys. Rev. B* 62 (2000), p. 1203. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.62.1203

276. **Billinge, S. J. L.**, R. G. DiFrancesco, M. F. Hundley, J. D. Thompson, and G. H. Kwei. "Competition between charge localization and delocalization in $La_{0.5}Ca_{0.5}MnO_3$". In: *Phys. Rev. Lett.* (2000). Unpublished

277. E. S. Božin, **Billinge, S. J. L.**, G. H. Kwei, and H. Takagi. "Local structural evidence for inhomogeneous charge distribution in CuO_2 planes of superconducting $La_{2-x}Sr_xCuO_4$". In: *Physica C* 341-348 (2000), p. 1793. URL: http://www.sciencedirect.com/science/article/pii/S0921453400010741

278. E. S. Božin, G. H. Kwei, H. Takagi, and **Billinge, S. J. L.** "Neutron diffraction evidence of microscopic charge inhomogeneities in the CuO_2 plane of superconducting $La_{2-x}Sr_xCu_4$ $(0 \leq x \leq 0.30)$". In: *Phys. Rev. Lett.* 84 (2000), pp. 5856–5859. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.84.5856

279. M. Gutmann, **Billinge, S. J. L.**, E. Brosha, and G. H. Kwei. "Local structural evidence for charge inhomogeneities in the CuO_2 planes of $YBa_2Cu_3O_{6+x}$ (x=0.25, 0.45, 0.65, 0.94)". In:

Physica C 341-348 (2000), p. 2143. DOI: 10.1016/S0921-4534(00)01094-7. URL: http://www.sciencedirect.com/science/article/pii/S0921453400010947

280. M. Gutmann, **Billinge, S. J. L.**, E. L. Brosha, and G. H. Kwei. "Possible charge inhomogeneities in the CuO_2 planes of $YBa_2Cu_3O_{6+x}$ (x=0.25, 0.45, 0.65, 0.94) from pulsed neutron diffraction". In: *Phys. Rev. B* 61 (2000), p. 11762. DOI: 10.1103/PhysRevB.61.11762. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.61.11762

281. V. Petkov, **Billinge, S. J. L.**, J. Heising, and M. G. Kanatzidis. "Application of atomic pair distribution function analysis to materials with intrinsic disorder. Three-dimensional structure of exfoliated-restacked WS_2: not just a random turbostratic assembly of layers". In: *J. Am. Chem. Soc.* 122 (2000), p. 11571. URL: http://pubs.acs.org/doi/abs/10.1021/ja002048i

282. V. Petkov, I-K. Jeong, F. Mohiuddin-Jacobs, Th. Proffen, and **Billinge, S. J. L.** "Local structure of $In_{0.5}Ga_{0.5}As$ from joint high-resolution and differential pair distribution function analysis". In: *J. Appl. Phys.* 88 (2000), p. 665. URL: http://scitation.aip.org/content/aip/journal/jap/88/2/10.1063/1.373718

283. V. Petkov, **Billinge, S. J. L.**, S. D. Shastri, and B. Himmel. "High-resolution atomic distribution functions of disordered materials by high-energy X-ray diffraction". In: *J. Non-Crystalline Solids* 293-295 (2000), p. 726. URL: http://www.sciencedirect.com/science/article/pii/S002230930100864X

284. V. Petkov, **Billinge, S. J. L.**, J. Heising, M. G. Kanatzidis, S. D. Shastri, and S. Kycia. "High real-space resolution structure of materials by high-energy X-ray diffraction". In: *Mater. Res. Soc. Symp. Proc.* 590 (2000), p. 151. URL: https://www.cambridge.org/core/journals/mrs-online-proceedings-library-archive/article/high-real-space-resolution-structure-of-materials-by-high-energy-x-ray-diffraction/DDC148B6CDABB14D08804D71E1E500B2

285. V. Petkov, **Billinge, S. J. L.**, S. D. Shastri, and B. Himmel. "Polyhedral units and network connectivity in calcium aluminosilicate glasses from high energy X-ray diffraction". In: *Phys. Rev. Lett.* 85 (2000), p. 3436. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.85.3436

286. M. Wachhold, K. Kasthuri Rangan, **Billinge, S. J. L.**, V. Petkov, J. Heising, and M. G. Kanatzidis. "Mesostructured non-oxidic solids with adjustable worm-hole shaped pores: M-Ge-Q (Q=S, Se) frameworks based on tetrahedral $[Ge_4Q_{10}]^{4-}$ clusters". In: *Advanced Mater.* 12 (2000), p. 85. URL: http://onlinelibrary.wiley.com/doi/10.1002/(SICI)1521-4095(200001)12:2%3C85::AID-ADMA85%3E3.0.CO;2-P/full

287. M. Wachhold, K. K. Rangan, M. Lei, M. F. Thorpe, **Billinge, S. J. L.**, V. Petkov, J. Heising, and M. G. Kanatzidis. "Mesostructured metal germanium sulphide and selenide materials based on the tetrahedral $[Ge_4S_{10}]^{4-}$ and $[Ge_4Se_{10}]^{4-}$ units: Surfactant templated three-dimensional disordered frameworks perforated with worm-holes". In: *J. Solid State Chem.* 152 (2000), p. 21. URL: http://www.sciencedirect.com/science/article/pii/S0022459600986730

288. M. Acharya, M. S. Strano, J. P. Matthews, **Billinge, S. J. L.**, V. Petkov, S. Subramoney, and H. C. Foley. "Simulation of nanoporous carbons: a chemically constrained structure". In: *Philos. Mag. B* 79 (1999), p. 1499. URL: http://www.tandfonline.com/doi/abs/10.1080/13642819908218318

289. J. F. Bardeau, A. S. Eberhardt, B. Scott, **Billinge, S. J. L.**, S. Kycia, T. Egami, and B. I. Swanson. "Recent structural studies of PtI". in: *Synthetic Metals* 103 (1999), p. 2596. URL: http://www.sciencedirect.com/science/article/pii/S0379677998006559

290. **Billinge, S. J. L.** "Polarons in manganites: now you see them, now you don't". In: *Physics of Manganites*. Ed. by T. A. Kaplan and S. D. Mahanti. New York: Klewer Academic/Plenum, 1999, p. 201. URL: http://link.springer.com/chapter/10.1007/0-306-47091-8_12#page-1

291. **Billinge, S. J. L.**, V. Petkov, Th. Proffen, G. H. Kwei, J. L. Sarrao, S. D. Shastri, and S. Kycia. "Charge inhomogeneities in the colossal magnetoresistant manganites from the local atomic structure". In: *Mater. Res. Soc. Symp. Proc.* 602 (1999), p. 177. DOI: 10.1557/PROC-602-177. URL: http://dx.doi.org/10.1557/PROC-602-177

292. E. S. Božin, **Billinge, S. J. L.**, G. H. Kwei, and H. Takagi. "Charge-stripe ordering from local octahedral tilts: underdoped and superconducting $La_{2-x}Sr_xCuO_4$ ($\mathbf{0 \leq x \leq 0.3}$)". In: *Phys. Rev. B* 59 (1999), p. 4445. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.59.4445

293. I. -K. Jeong, Th. Proffen, F. Mohiuddin-Jacobs, and **Billinge, S. J. L.** "Measuring correlated atomic motion using X-ray diffraction". In: *J. Phys. Chem. A* 103 (1999), pp. 921–924. DOI: 10.1021/jp9836978. URL: http://pubs.acs.org/doi/abs/10.1021/jp9836978

294. Thomas R. Pauly, Yu Liu, Thomas J. Pinnavaia, **Billinge, Simon J. L.**, and Thomas P. Rieker. "Textural mesoporosity and the catalytic activity of mesoporous molecular sieves with wormhole framework structures". In: *J. Am. Chem. Soc.* 38 (1999), p. 8835. URL: http://pubs.acs.org/doi/abs/10.1021/ja991400t

295. V. Petkov, R. G. DiFrancesco, **Billinge, S. J. L.**, M. Acharya, and H. C. Foley. "Local structure of nanoporous carbons". In: *Philos. Mag. B* 79 (1999), p. 1519. URL: http://www.tandfonline.com/doi/abs/10.1080/13642819908218319

296. V. Petkov, I. -K. Jeong, J. S. Chung, M. F. Thorpe, S. Kycia, and **Billinge, S. J. L.** "High real-space resolution measurement of the local structure of $Ga_{1-x}In_xAs$ using X-ray diffraction". In: *Phys. Rev. Lett.* 83.20 (1999), pp. 4089–4092. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.83.4089

297. Th. Proffen and **Billinge, S. J. L.** "PDFFIT, a program for full profile structural refinement of the atomic pair distribution function". In: *J. Appl. Crystallogr.* 32 (1999), pp. 572–575. DOI: 10.1107/S0021889899003532. URL: http://journals.iucr.org./j/issues/1999/03/00/gl0603/gl0603.pdf

298. Th. Proffen, R. G. DiFrancesco, **Billinge, S. J. L.**, E. L. Brosha, and G. H. Kwei. "Measurement of the local Jahn-Teller distortion in $LaMnO_{3.006}$". In: *Phys. Rev. B* 60 (1999), p. 9973. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.60.9973

299. K. Kasthuri Rangan, **Billinge, Simon J. L.**, Valeri Petkov, Joy Heising, and Mercouri G. Kanatzidis. "Aqueous Mediated Synthesis of Mesostructured Manganese Germanium Sulfide with Hexagonal Order". In: *Chem. Mater* 11 (1999), p. 2629. URL: http://pubs.acs.org/doi/abs/10.1021/cm990456j

300. **Billinge, S. J. L.** "Real-space Rietveld: full profile structure refinement of the atomic pair distribution function". In: *Local Structure from Diffraction*. Ed. by S. J. L. Billinge and M. F. Thorpe. New York: Plenum, 1998, p. 137

301. E. S. Božin, **Billinge, S. J. L.**, and G. H. Kwei. "Reexamination of the second order structural phase transition in $La_{2-x}A_xCuO_4$ (A=Ba,Sr)". In: *Physica B* 241-243 (1998), p. 795. URL: http://www.sciencedirect.com/science/article/pii/S0921452697007205

302. E. S. Božin and **Billinge, S. J. L.** "Understanding the role of the local structure in the second order structural phase transition of $La_{2-x}A_xCuO_4$ (A=Ba,Sr)". In: *Solid State Phenomena* 61-62 (1998), p. 271. URL: http://www.scientific.net/SSP.61-62.271

303. K. S. Choi, R. Patschke, **Billinge, S. J. L.**, M. J. Waner, M. Dantus, and M. G. Kanatzidis. "Charge density wave caused by reducing $ThSe_3$ by on electron. Superstructure and short-range order in ATh_2Se_6 (A=K, Rb) studied by X-ray diffraction, electron diffraction and diffuse scattering". In: *J. Am. Chem. Soc.* 120 (1998), p. 10706. URL: http://pubs.acs.org/doi/abs/10.1021/ja981675t

304. R. G. DiFrancesco, **Billinge, S. J. L.**, G. H. Kwei, J. J. Neumeier, and J. D. Thompson. "Local structure and polaron formation in $La_{1-x}Ca_xMnO_3$". In: *Physica B* 241-243 (1998), p. 421. URL: http://www.sciencedirect.com/science/article/pii/S092145269700608X

305. G. H. Kwei, D. Louca, **Billinge, S. J. L.**, and H. D. Rosenfeld. "Recent "Local" structural studies: Metallic Alloys, Superconductors and Proteins". In: *Local Structure from Diffraction.* Ed. by S. J. L. Billinge and M. F. Thorpe. New York: Plenum, 1998, p. 323

306. M. F. Thorpe, J. S. Chung, **Billinge, S. J. L.**, and F. Mohiuddin-Jacobs. "Advances in pair distribution profile fitting in alloys". In: *Local Structure from Diffraction.* Ed. by S. J. L. Billinge and M. F. Thorpe. New York: Plenum, 1998, p. 157. URL: http://link.springer.com/chapter/10.1007%2F0-306-47077-2_9

307. A. P. Wilkinson, J. Xu, S. Pattanaik, and **Billinge, S. J. L.** "Neutron scattering studies of compositional heterogeneity in sol-gel processed PZT $(PbZr_{0.5}Ti_{0.5})O_3$". In: *Chem. Mater.* 10 (1998), p. 3611. URL: http://pubs.acs.org/doi/abs/10.1021/cm980368j

308. **Billinge, S. J. L.** "Electronic Oxides: Properties and applications". In: *CFMR* (1997). Web Proceedings of the 11th Annual CFMR symposium, published in conjunction with the Virtual University at Michigan State University

309. T. Egami, **Billinge, S. J. L.**, S. Kycia, W. Dmowski, and A. S. Eberhardt. "Information stored in high Q-space: role of high energy scattering". In: *AIP Conf. Series* 417 (1997), p. 209. DOI: 10.1063/1.54573. URL: http://scitation.aip.org/content/aip/proceeding/aipcp/10.1063/1.54573

310. G. H. Kwei, D. N. Argyriou, **Billinge, S. J. L.**, A. C. Lawson, J. J. Neumeier, A. P. Ramirez, M. A. Subramanian, and J. D. Thompson. "Lattice effects in perovskite and pyrochlore CMR materials". In: *Mat. Res. Soc. Symp. Proc.* 475 (1997), p. 533. DOI: 10.1557/PROC-475-533. URL: https://www.cambridge.org/core/journals/mrs-online-proceedings-library-archive/article/lattice-effects-in-perovskite-and-pyrochlore-cmr-materials/781DD64BB49C2AD41E77901CEC8782F3

311. **Billinge, S. J. L.** "The structure of real materials using X-ray and neutron scattering". In: *Current Opinion in Solid State and Mater. Sci.* 1.4 (1996), p. 477. URL: http://www.sciencedirect.com/science/article/pii/S1359028696800611

312. **Billinge, S. J. L.** and G. H. Kwei. "Probing the short-range order and dynamics of phase transition using neutron powder diffraction". In: *J. Phys. Chem. Solids* 57 (1996), p. 1457. URL: http://www.sciencedirect.com/science/article/pii/0022369796000133

313. **Billinge, S. J. L.**, R. G. DiFrancesco, G. H. Kwei, J. J. Neumeier, and J. D. Thompson. "Direct observation of lattice polaron formation in the local structure of $La_{1-x}Ca_xMnO_3$". In: *Phys. Rev. Lett.* 77 (1996), pp. 715–718. DOI: 10.1103/PhysRevLett.77.715. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.77.715

314. T. Egami and **Billinge, S. J. L.** "Lattice Effects in high-T_c superconductors". In: *Physical properties of high-temperature superconductors V.* ed. by D. M. Ginsberg. Singapore: World–Scientific, 1996, pp. 265–373

315. M. S. Kane, J. F. Goellner, H. C. Foley, R. G. DiFrancesco, **Billinge, S. J. L.**, and L. F. Allard. "Symmetry breaking in nanostructure development of carbogenic molecular sieves: effects of morphological pattern formation on oxygen and nitrogen transport". In: *Chem. Mater.* 8 (1996), p. 2159. URL: http://pubs.acs.org/doi/abs/10.1021/cm960085w

316. **Billinge, S. J. L.** and G. H. Kwei. "Determination of the Local Atomic Structure of $La_{2-x}(Sr,Ba)_xCuO_4$ Materials From Neutron Powder Diffraction Data". In: *Mater. Res. Soc. Proc.* 376 (1995). Ed. by D. A. Neumann, T. P. Russell, and B. J. Wuensch, p. 523

317. G. H. Kwei, **Billinge, S. J. L.**, S. W. Cheong, and J. G. Saxton. "Pair-distribution functions of ferroelectric perovskites: direct observation of structural gound-states". In: *Ferroelectrics* 164 (1995), p. 57. URL: http://www.tandfonline.com/doi/abs/10.1080/00150199508221830

318. **Billinge, S. J. L.**, G. H. Kwei, and J. D. Thompson. "Experimental evidence for lattice effects in high temperature superconductors". In: *Strongly Correlated Electronic Materials*. Ed. by K. Bedell. New York: Addison Wesley, 1994

319. **Billinge, S. J. L.**, G. H. Kwei, and H. Takagi. "Local Structure and Superconductivity in $La_{2-x}(Sr,Ba)_xCuO_4$ for x = 0.125 and x = 0.15". In: *Physica B* 199-200 (1994), p. 244

320. **Billinge, S. J. L.**, G. H. Kwei, and H. Takagi. "Structural ground-state of La_2CuO_4 in the LTO phase: evidence of local disorder". In: *Physica C* 235-240 (1994), p. 1281. URL: http://www.sciencedirect.com/science/article/pii/0921453494918651

321. **Billinge, S. J. L.**, G. H. Kwei, and H. Takagi. "Local octahedral tilts in $La_{2-x}Ba_xCuO_4$: evidence for a new structural length scale". In: *Phys. Rev. Lett.* 72 (1994), p. 2282. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.72.2282

322. T. Egami and **Billinge, S. J. L.** "Lattice effects in high-temperature superconductors". In: *Prog. Mater. Sci.* 38 (1994), p. 359. URL: http://repository.upenn.edu/dissertations/AAI9712974/

323. **Billinge, S. J. L.** and T. Egami. "Short-range atomic structure of $Nd_{2-x}Ce_xCuO_{4-y}$ determined by real-space refinement of neutron-powder-diffraction data". In: *Phys. Rev. B* 47 (1993), p. 14386. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.47.14386

324. **Billinge, S. J. L.**, G. H. Kwei, A. C. Lawson, J. D. Thompson, and H. Takagi. "Superconductivity and the low-temperature orthorhombic to tetragonal phase transition in $La_{2-x}Ba_xCuO_4$". In: *Phys. Rev. Lett.* 71 (1993), p. 1903. URL: http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.71.1903

325. T. Egami and **Billinge, S. J. L.** "Local lattice distortion and mechanism of superconductivity". In: *Advances in Superconductivity*. Ed. by Y. Bando and H. Yamauchi. Tokyo: Springer Verlag, 1993. URL: http://link.springer.com/chapter/10.1007/978-4-431-68305-6_13

326. G. H. Kwei, A. C. Lawson, **Billinge, S. J. L.**, and S. W. Cheong. "Structures of the ferroelectric phases of barium titanate". In: *J. Phys. Chem.* 97 (1993), p. 2368. URL: http://pubs.acs.org/doi/abs/10.1021/j100112a043

327. **Billinge, S. J. L.** and T. Egami. "Local structural changes in high-Tc oxides associated with superconductivity". In: *Lattice Effects in High T_c Superconductors*. Ed. by Y. Bar-Yam, T. Egami, J. Mustre-de Leon, and A. R. Bishop. Singapore: World Scientific, 1992, p. 93

328. **Billinge, S. J. L.** "Local atomic structure and superconducivity of $Nd_{2-x}Ce_xCuO_{4-y}$: a pair distribution function study". Ph.D Thesis, 1992

329. T. Egami, B. H. Toby, **Billinge, S. J. L.**, Chr. Janot, J. D. Jorgensen, D. G. Hinks, M. K. Crawford, W. E. Farneth, and E. M. McCarron. "Local Structural anomaly at Tc observed by neutron scattering". In: *High Temperature Superconductivity: Physical Properties, Microscopic Theory and Mechanisms*. Ed. by J. Ashkenazi et al. New York: Plenum, 1992

330. **Billinge, S. J. L.**, P. K. Davies, T. Egami, and C. R. A. Catlow. *Out of phase displacements of oxygen from the CuO_2 sheets in $Ca_{0.85}Sr_{0.15}CuO_2$ by atom-pair distribution function analysis*. Ed. by Y. Bar-Yam, T. Egami, Mustre de Leon J., and A. R. Bishop. Gaithersburg: NIST, 1991

331. **Billinge, S. J. L.**, T. Egami, D. R. Richards, D. G. Hinks, B. Dabrowski, J. D. Jorgensen, and K. J. Volin. "Local structural change close to Tc in $Nd_{1.835}Ce_{0.165}CuO_4$". In: *Physica C* 179 (1991), p. 279. URL: http://www.sciencedirect.com/science/article/pii/0921453491921728

332. **Billinge, S. J. L.**, P. K. Davies, T. Egami, and C. R. A. Catlow. "Deviations from planarity of copper-oxygen sheet in $Ca_{0.85}Sr_{0.15}CuO_2$". In: *Phys. Rev. B* 43 (1991), p. 10340. URL: http://journals.aps.org/prb/abstract/10.1103/PhysRevB.43.10340

333. T. Egami, B. H. Toby, **Billinge, S. J. L.**, H. D. Rosenfeld, J. D. Jorgensen, D. G. Hinks, B. Dabrowski, M. A. Subramanian, M. K. Crawford, W. E. Farneth, and D. M. McCarron. "Local structural anomaly near T_c observed by pulsed neutron scattering". In: *Physica C* 185-189 (1991), p. 867. URL: http://www.sciencedirect.com/science/article/pii/092145349191657P

334. T. Egami, B. H. Toby, W. Dmowski, **Billinge, S. J. L.**, P. K. Davies, J. D. Jorgensen, M. A. Subramanian, and A. W. Sleight. "Symmetry breaking oxygen displacements in superconducting oxides". In: *Physica C* 162-164 (1989), p. 93. URL: http://www.sciencedirect.com/science/article/pii/0921453489909337