

# Long Yang

Assistant Professor

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## RESEARCH INTERESTS

My research focuses on the study of local structure-property relationship in crystalline, non-crystalline, and nanocrystalline materials at the sub-nanometer length scale using x-ray, neutron, and electron diffraction techniques, including atomic pair distribution function (PDF) and atomic electron tomography (AET) methods.

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## EDUCATION

<b>PhD in Materials Science and Engineering</b> , Columbia University, New York, USA	2017 - 2021
<b>MSc in Materials Science and Engineering</b> , Columbia University, New York, USA	2015 - 2016
<b>BSc in Optical Info Science and Technology</b> , Fudan University, Shanghai, China	2011 - 2015

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## APPOINTMENTS

<b>Assistant Professor</b> , School of Materials Science and Engineering, Tongji University, China	2022 - Now
<b>Postdoctoral Scholar</b> , Department of Physics and Astronomy, UCLA, USA	2021 - 2022
<b>Co-Advised Research Assistant</b> , Neutron Diffraction Group, ORNL, USA	2017 - 2020

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## HONORS & AWARDS

- Shanghai Leading Talents Program, 2021 (Overseas)
- WangDao Scholar, 2015 (Selected as one of the three distinguished projects at Fudan University)
- Fudan University Scholarship, 2013-2015 (Multiple times)
- National Scholarship, 2012 (Awarded by the Ministry of Education of the People's Republic of China)

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## TALKS & CONFERENCES

### Community Scientific Software Efforts:

- PDF in the Cloud (PDFfitc): A cloud-based diffraction data analysis platform at <https://pdfitc.org>.
- PDFgui: A local atomic structure modeling software for x-ray and neutron pair distribution function data (Current lead developer).
- Diffraction Data Pipeline: Time-of-light neutron powder diffraction auto data reduction, calibration, and fitting of Rietveld and PDF data collected at the NOMAD beamline of Spallation Neutron Source (SNS), Oak Ridge National Lab. A cloud-based platform is created to host some of these analysis tools at the ADvanced DIffraction Environment (<https://addie.ornl.gov>.)

### Journal Reviewers:

- ACS Applied Nano Materials, APL Materials, etc.

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## SCIENTIFIC ACTIVITIES

1. *The Structure-Property Relationship of Atomic Local Structures and Low Lattice Thermal Conductivities*, 14th Chinese Conference on Thermoelectric Materials and Applications (CCT2022), Tongxiang, Zhejiang, China, March 2023 (Oral presentation)
2. 2023 China Spallation Neutron Source (CSNS) User Meeting, The Institute of High Energy Physics (IHEP) of the Chinese Academy of Sciences (CAS), Dongguan, Guangdong, China, March 2023 (Attendee)
3. National Program on Key Research and Development 'Basic Research Conditions and Major Scientific Instruments and Equipment Research and Development' Key Projects 2023 Annual Progress Meeting (Scientific Data Section), Beijing, China, March 2023 (Invited committee members)
4. *Atomic Pair Distribution Function Data Processing for Total Scattering Experiments*, 3rd Advanced Light Source Neutron Source Scientific Data and Software Workshop, IHEP of CAS, Beijing, China, March 2023 (Oral presentation)
5. National Program on Key Research and Development 'The Structure-Property Relationship of Multiphase Catalysis Multi-Phase Based on Neutron Scattering and Spectroscopy' Project Promotion and Plan Validation Meeting, Beijing, China, February 2023 (Invited committee members)

6. 2022 Shanghai Soft X-Ray Free Electron Laser Instrument User Meeting, ShanghaiTech University, Shanghai, China, November 2022 (Attendee)
7. *Data Processing for Synchrotron X-ray and Neutron Experiments*, IHEP School of Computing 2022, IHEP of CAS, Beijing, China, August 2022 (Invited talk)
8. *Data Mining and High-Energy Diffraction Data Analysis in the Cloud*, IHEP Computed Center, High Energy Photon Source (HEPS), IHEP of CAS, Beijing, China, February 2022 (Invited talk)
9. *Structure-mining: An Automated Tool to Find Candidate Structures from Neutron and X-ray PDF Data*, PDF-2020 workshop, Remote, UK, China & USA, December 2020 (Invited talk)
10. *Structure-mining: An Automated Tool to Find Candidate Structures from Neutron and X-ray PDF Data*, 10th American Conference on Neutron Scattering (ACNS 2020), Remote, USA, July 2020 (Oral presentation)
11. *Towards Machine Learning on Experimental Nanostructure Data*, Columbia University Data Science Day 2020, New York, USA, March 2020 (Oral presentation, recorded at <https://youtu.be/8xwWrRUkhN4>)
12. *Introduction of DiffPy-CMI: What It Can Do Beyond PDFgui*, 2nd US School on Total Scattering Analysis, Oak Ridge, USA, August 2018 (Invited talk)
13. *Role of Local Structural Distortions on Mo and V Nitrides with The Pair Distribution Function Analysis*, Quantum Complex Matter 2018 (QCM 2018), Laboratori Nazionali di Frascati, Rome, Italy, June 2018 (Poster)

## PUBLICATIONS

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**Google Scholar:** <https://scholar.google.com/citations?user=H2mOKp8AAAAJ>

H-index=8, Citations=518 (Dated at April 2, 2023)

## Journal Articles and Books

- [1] Qi Tao, Chaogang Xing, Seungyeol Lee, Long Yang, Qingjin Zeng, Shangying Li, Tianqi Zhang, Guanglie Lv, Hongping He, and Komarneni Sridhar. Local Structure Determination of Zn-smectite, *Am. Mineral.*, September 2022. doi: 10.2138/am-2022-8591.
- [2] Emil T. S. Kjær, Olivia Aalling-Frederiksen, Long Yang, Nancy K. Thomas, Mikkel Juelsholt, Simon J. L. Billinge, and Kirsten M. Ø. Jensen. In Situ Studies of the Formation of Tungsten and Niobium Oxide Nanoparticles: Towards Automated Analysis of Reaction Pathways from PDF Analysis using the Pearson Correlation Coefficient, *Chem.-Methods*, 2(9):e202200034, August 2022. doi: 10.1002/cmtd.202200034.
- [3] Zachary Thatcher, Chia-Hao Liu, Long Yang, Brennan C. McBride, Gia Thinh Tran, Allison Wustrow, Martin A. Karlsen, James R. Neilson, Dorthe B. Ravnsbæk, and Simon J. L. Billinge. nmfMapping: A cloud-based web application for non-negative matrix factorization of powder diffraction and pair distribution function datasets, *Acta Cryst. A*, 78(3):242–248, May 2022. doi: 10.1107/S2053273322002522.
- [4] Simon J. L. Billinge, Sandra H. Skjærvø, Maxwell W. Terban, Songsheng Tao, Long Yang, Yevgeny Rakita, and Benjamin A. Frandsen. Local structure determination using total scattering data. In *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*. Elsevier, January 2021.
- [5] 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, *Acta Cryst. A*, 77(1):2–6, January 2021. doi: 10.1107/S2053273320013066.
- [6] Muhammad Boota, Tanveer Hussain, Long Yang, Matthieu Bécuwe, William Porzio, Luisa Barba, and Rajeev Ahuja. Mechanistic Understanding of the Interactions and Pseudocapacitance of Multi-Electron Redox Organic Molecules Sandwiched between MXene Layers, *Adv. Electron. Mater.*, 7(4):2001202, 2021. doi: 10.1002/aelm.202001202.
- [7] 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<sub>2</sub>O<sub>4</sub>, *Phys. Rev. B*, 102(23):235128, December 2020. doi: 10.1103/PhysRevB.102.235128.

- [8] Muhammad Boota, Chi Chen, Long Yang, Alexander I. Kolesnikov, Naresh C. Osti, William Porzio, Luisa Barba, and Jianjun Jiang. Probing Molecular Interactions at MXene–Organic Heterointerfaces, *Chem. Mater.*, 32(18):7884–7894, September 2020. doi: 10.1021/acs.chemmater.0c02662.
- [9] Long Yang, Pavol Juhás, Maxwell W. Terban, Matthew G. Tucker, and Simon J. L. Billinge. Structure-mining: Screening structure models by automated fitting to the atomic pair distribution function over large numbers of models, *Acta Cryst. A*, 76(3):395–409, May 2020. doi: 10.1107/S2053273320002028.
- [10] 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, *Adv. Mater.*, 31(33):1902393, June 2019. doi: 10.1002/adma.201902393.
- [11] Alexander P. Aydt, Boyu Qie, Andrew Pinkard, Long Yang, Qian Cheng, Simon J. L. Billinge, Yuan Yang, and Xavier Roy. Microporous Battery Electrodes from Molecular Cluster Precursors, *ACS Appl. Mater. Interfaces*, 11(12):11292–11297, March 2019. doi: 10.1021/acsami.8b18149.
- [12] Wei Cao, Long Yang, Stéphane Auffret, and William E. Bailey. Nearly isotropic spin-pumping related Gilbert damping in Pt/Ni<sub>81</sub>Fe<sub>19</sub>/Pt, *Phys. Rev. B*, 99(9):094406, March 2019. doi: 10.1103/PhysRevB.99.094406.
- [13] Xu Xiao, Patrick Urbankowski, Kanit Hantanasirisakul, Yao Yang, Stephen Sasaki, Long Yang, Chi Chen, Hao Wang, Ling Miao, Sarah H. Tolbert, Simon J. L. Billinge, Héctor D. Abruña, Steven J. May, and Yury Gogotsi. Scalable Synthesis of Ultrathin Mn<sub>3</sub>N<sub>2</sub> Exhibiting Room-Temperature Antiferromagnetism, *Adv. Funct. Mater.*, 29(17):1809001, March 2019. doi: 10.1002/adfm.201809001.
- [14] Julien Lombardi, Long Yang, Frederick A. Pearsall, Nasim Farahmand, Zheng Gai, Simon J. L. Billinge, and Stephen O’Brien. Stoichiometric Control over Ferroic Behavior in Ba(Ti<sub>1-x</sub>Fe<sub>x</sub>)O<sub>3</sub> Nanocrystals, *Chem. Mater.*, 31(4):1318–1335, February 2019. doi: 10.1021/acs.chemmater.8b04447.
- [15] Patrick Urbankowski, Babak Anasori, Kanit Hantanasirisakul, Long Yang, Lihua Zhang, Bernard Haines, Steven J. May, Simon J. L. Billinge, and Yury Gogotsi. 2D molybdenum and vanadium nitrides synthesized by ammoniation of 2D transition metal carbides (MXenes), *Nanoscale*, 9(45):17722–17730, November 2017. doi: 10.1039/C7NR06721F.