Long Yang

Assistant Professor

School of Materials Sceince and Engineering, Tongji University, Shanghai 201804, China

long_yang@tongji.edu.cn | https://www.yanglonggroup.com

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.

Education

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

Appointments

Assistant Professor, School of Materials Science and Engineering, Tongji University, China 2022.07 - Now
Postdoctoral Scholar, Department of Physics and Astronomy, UCLA, USA 2022.01 - 2022.07
Co-Advised Research Assistant, Neutron Diffraction Group, ORNL, USA 2017.06 - 2020.06

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)

Professional Activities

Community Scientific Software Efforts:

- PDF in the Cloud (PDFitc): cloud-based diffraction data analysis platform at https://pdfitc.org.
- PDFgui: local structure modeling program for pair distribution function data (Current lead developer).
- Diffraction Data Pipeline: time-of-light neutron diffraction auto data reduction, calibration, and fitting of Rietveld and PDF refinements for NOMAD beamline at Spallation Neutron Source (SNS), Oak Ridge National Lab.

Journal Reviewers:

- ACS Applied Nano Materials

Dissertation Committee:

- Guanjie Zhang, PhD (Advisor: Nan Zhang, Xi'an Jiaotong University, 2023.02)

Conferences

1. *Data Processing for Synchrotron X-ray and Neutron Experiments,* IHEP School of Computing 2022, The Institute of High Energy Physics (IHEP) of the Chinese Academy of Sciences, Beijing, China, Aug 2022 (Invited talk)
2. *Data Mining and High-Energy Diffraction Data Analysis in the Cloud,* IHEP Computed Center, High Energy Photon Source (HEPS), The Institute of High Energy Physics (IHEP) of the Chinese Academy of Sciences, Beijing, China, Feb 2022 (Invited talk)
3. *Structure-mining: An Automated Tool to Find Candidate Structures from Neutron and X-ray PDF Data,* PDF-2020 workshop, Remote, UK, China & USA, Dec 2020 (Invited talk)
4. *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)
5. *Towards Machine Learning on Experimental Nanostructure Data,* Columbia University Data Science Day 2020, New York, USA, Mar 2020 (Oral presentation, recorded at https://youtu.be/8xwWrRUkhN4)
6. *Introduction of DiffPy-CMI: What It Can Do Beyond PDFgui,* 2nd US School on Total Scattering Analysis, Oak Ridge, USA, Aug 2018 (Invited talk)
7. *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

Google Scholar: https://scholar.google.com/citations?user=H2mOKp8AAAAJ
H-index=8, Citations=494 (Dated at February 10, 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 $MgTi_2O_4$, *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 $Pt/Ni_{81}Fe_{19}/Pt$, *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_3N_2 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 $Ba(Ti_{1-x}Fe_x)O_3$ 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.