

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 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 Information Science and Technology , Fudan University, Shanghai, China	2011 - 2015

APPOINTMENTS

Assistant Professor , School of Materials Science and Engineering, Tongji University, China	2022 - Now
Postdoctoral Scholar , Department of Physics and Astronomy, UCLA, USA	2021 - 2022

HONORS & AWARDS

- Outstanding Mentor at the Tongji University Student Innovation Base, 2023 (Awarded by the School of Innovation and Entrepreneurship at Tongji University)
- 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)

SCIENTIFIC ACTIVITIES

Community Scientific Software Efforts:

- PDF in the Cloud (PDFitc): 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).
- ADvanced DIffraction Environment (ADDIE): A cloud-based platform at the Oak Ridge National Laboratory to host neutron diffraction data analysis tools at <https://addie.ornl.gov>.
- Diffraction Data Pipeline: time-of-flight neutron diffraction data auto reduction, calibration, and structural fitting of diffraction and PDF datasets collected at the NOMAD beamline of Spallation Neutron Source (SNS).

Committee Members:

- One of the first committee members of the local structure and total scattering technique committee of the Chinese Crystallographic Society (IUCr, CCRS), which was founded in October 2023.
- International large scientific facility user proposal reviewer: Shanghai Synchrotron Radiation Facility (SSRF), Japan Proton Accelerator Research Complex (J-PARC).

Journal Reviewers:

- Science Advances, Acta Materialia, APL Materials, ACS Applied Nano Materials, etc.

TEACHING

- Solid State Physics, 2023 Fall (Graduate)
- Material Science Major Experiments, 2023 Fall, 2024 Fall (Undergraduate)
- Fundamentals of Materials Science, 2024 Fall (Undergraduate)
- Material Physics, 2024 Fall (Undergraduate)

TALKS & CONFERENCES

1. *Local Structures of Materials and Atomic Pair Distribution Function*, Sino-French Colloquium Energy Materials for Sustainable Development, Tongji University, Shanghai, May 2025 (Oral Talk)
2. *Atomic Local Structures and Pair Distribution Function*, Harbin Institute of Technology, Shenzhen, Guangdong, December 2024 (Invited Talk)
3. *PDF Local Structure Characterization and Chemical Short-Range Ordering*, The 13th China Congress on Particle Technology, Suzhou, Jiangsu, China, October 2024 (Invited Talk)
4. *Atomic Local Structures and Low Lattice Thermal Conductivity Materials*, The 16th Chinese Conference on Thermoelectric Materials and Applications, Chongqing, China, October 2024 (Invited Talk)
5. *PDF Local Structure Generative Model Algorithms*, Committee Member Meeting of the Local Structure and Total Scattering Technique Committee of the Chinese Crystallographic Society, Xining, Qinghai, China, July 2024 (Invited Talk, Committee Member)
6. *The Atomic Local Structure Characterization on Materials*, Suzhou Laboratory, Suzhou, Jiangsu, China, June 2024 (Invited Talk)
7. *The Development of Light Sources and Experimental Methods*, 2024 Spring Semester Nanjing University of Science And Technology International Course on the Introduction to Synchrotron Radiation and Neutron Scattering, Remote, China, May 2024 (Invited Talk)
8. National Key Research and Development Program of China 'Study on the Synchrotron Radiation High-Throughput Characterization of Novel Actinide Alloys' 2024 Mid-term Review Meeting, Shanghai, China, April 2024 (Invited Committee Member)
9. National Key Research and Development Program of China 'Study on the Structure-Property Relationship of Multiphase Catalysis Based on Neutron Scattering and Spectroscopy' 2023 Annual Work Summary Meeting, Dongguan, Guangdong, China, January 2024 (Invited Committee Member)
10. *Unveiling local magnetic correlations: the development of magnetic pair distribution function at CSNS*, The 24th meeting of The International Collaboration of Advanced Neutron Sources (ICANS XXIV), Dongguan, Guangdong, China, October 2023 (Invited Talk)
11. *The cloud platform for PDF data analysis of local structure characterization*, The 9th Chinese Crystallographic Society (CCrS) meeting, Fuzhou, Fujian, China, October 2023 (Invited Talk, Committee Member)
12. 2023 China Spallation Neutron Source (CSNS) Multi-Physics Instrument User Meeting, Xining, Qinghai, China, August 2023 (Attendee)
13. *Data Processing for Advanced Light Source Experiments*, IHEP School of Computing 2023, IHEP of CAS, Beijing, China, August 2023 (Invited talk)
14. *The cloud platform for PDF data analysis of local structure characterization*, Chinese Materials Conference 2022-2023 by Chinese Materials Research Society(C-MRS), Shenzhen, Guangdong, China, July 2023 (Outstanding talk award)
15. *The Structure-Property Relationship of Atomic Local Structures and Low Lattice Thermal Conductivities*, The 14th Chinese Conference on Thermoelectric Materials and Applications (CCT2022), Tongxiang, Zhejiang, China, March 2023 (Oral presentation)
16. 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)
17. 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)
18. *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)
19. National Key Research and Development Program of China 'Study on the Structure-Property Relationship of Multiphase Catalysis Based on Neutron Scattering and Spectroscopy' Project Initiation and Implementation Plan Demonstration Meeting, Beijing, China, February 2023 (Invited committee members)
20. *The Atomic Local Structure Characterization on Materials*, Seminar at The State Key Lab of High Performance Ceramics and Superfine Microstructure Shanghai, Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China, December 2022 (Invited talk)

21. 2022 Shanghai Soft X-Ray Free Electron Laser Instrument User Meeting, ShanghaiTech University, Shanghai, China, November 2022 (Attendee)
22. *Data Processing for Synchrotron X-ray and Neutron Experiments*, IHEP School of Computing 2022, IHEP of CAS, Beijing, China, August 2022 (Invited talk)
23. *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)
24. *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)
25. *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)
26. *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/8xwWrUkhN4>)
27. *Introduction of DiffPy-CMI: What It Can Do Beyond PDFgui*, 2nd US School on Total Scattering Analysis, Oak Ridge, USA, August 2018 (Invited talk)
28. *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=12, Citations=900 (Dated at May 11, 2025)

Journal Articles and Books

- [1] Shasha Guo, Mohamed Ait Tamerd*, Changyuan Li, Xinyue Shi, Menghao Yang, Jingrong Hou, Jie Liu, Mingxue Tang, Shu-Chih Haw, Chien-Te Chen, Ting-Shan Chan, Chang-Yang Kuo, Zhiwei Hu, Long Yang*, and Jiwei Ma*. Activating Sodium Intercalation in Cation-Deficient Fe₃O₄ Through Mo Substitution, *Small*, 21(18):2408212, March 2025. doi: 10.1002/sml.202408212.
- [2] Heng Liu*, Long Yang*, Ting Shen, Changyuan Li, Te Kang, Huanhuan Niu, Wei-Hsiang Huang, Chun-Chi Chang, Menghao Yang, Guozhong Cao, and Chaofeng Liu. Distorting Local Structures to Modulate Ligand Fields in Vanadium Oxide for High-Performance Aqueous Zinc-Ion Batteries, *ACS Nano*, 19(9):9132–9143, March 2025. doi: 10.1021/acsnano.4c18250.
- [3] Di Zhang, Min Liu, Tao Jin, Long Yang*, Wen Li*, and Yanzhong Pei*. (AgSbTe₂)_{1-x}(Bi₂Te₃)_x-based thermoelectric device for low-grade heat recovery, *Mater. Today Phys.*, 52:101692, March 2025. doi: 10.1016/j.mtphys.2025.101692.
- [4] Shanshan Hu, Min Liu, Long Yang, Zhiwei Chen, Jun Luo, Wen Li, and Yanzhong Pei. Effective diffusion barrier layer enables a robust CdSb-based thermoelectric single-leg device, *J. Power Sources*, 630:236102, February 2025. doi: 10.1016/j.jpowsour.2024.236102.
- [5] Hyderkhan Renuka, Morgan Chen, Shwetha Sunil Kumar, Long Yang, Michael T. Lanagan, Sanjit Ghose, and B. Reeja-Jayan. Energy-efficient synthesis of Ti₃C₂T_x MXene for electromagnetic shielding, *Mater. Sci. Semicond. Process.*, 185:108966, January 2025. doi: 10.1016/j.mssp.2024.108966.
- [6] Xia Qi, Te Kang, Long Yang, Xinyue Zhang, Jun Luo, Wen Li, and Yanzhong Pei. Simultaneous Suppression of Phonon Transport and Carrier Concentration for Efficient Rhombohedral GeTe Thermoelectric, *Adv. Sci.*, 11(47):2407413, December 2024. doi: 10.1002/advs.202407413.
- [7] Long Yang*, Te Kang, Juping Xu*, and Wen Yin. Unveiling Short-Range Magnetic Correlations: The Development of Magnetic Pair Distribution Function Method at CSNS, *Nucl. Instrum. Methods Phys. Res. A*, 1069:169967, December 2024. doi: 10.1016/j.nima.2024.169967.
- [8] Yixin Hu, Xinyi Shen, Zhiwei Chen, Min Liu, Xinyue Zhang, Long Yang, Jun Luo, Wen Li, and Yanzhong Pei. Superior bendability enabled by inherent in-plane elasticity in Bi₂Te₃ thermoelectrics, *Mater. Today Phys.*, 48:101570, November 2024. doi: 10.1016/j.mtphys.2024.101570.

- [9] Tao Jin*, Long Yang*, Di Zhang, Xiaoyu Yang, Xinyue Zhang, Te Kang, Binghui Ge, Pengfei Nan, Wen Li, and Yanzhong Pei. Designing Semiconductors from the Assembly of Close-Packed Slabs, *Chem. Mater.*, 36(22):11189–11199, November 2024. doi: 10.1021/acs.chemmater.4c02062.
- [10] Heng Liu, Huanhuan Niu, Wei-Hsiang Huang, Ting Shen, Changyuan Li, Chun-Chi Chang, Menghao Yang, Chenlong Gao, Long Yang, Quan Zong, Yanzhong Pei, Guozhong Cao, and Chaofeng Liu. Unveiling the Local Structure and the Ligand Field of Organic Cation Preintercalated Vanadate Cathode for Aqueous Zinc-Ion Batteries, *ACS Energy Lett.*, 9(11):5492–5501, October 2024. doi: 10.1021/acsenergylett.4c02709.
- [11] Huanhuan Niu, Heng Liu, Long Yang, Te Kang, Ting Shen, Bingqi Jiang, Wei-Hsiang Huang, Chun-Chi Chang, Yanzhong Pei, Guozhong Cao, and Chaofeng Liu. Impacts of distorted local chemical coordination on electrochemical performance in hydrated vanadium pentoxide, *Nat. Commun.*, 15(1):9421, October 2024. doi: 10.1038/s41467-024-53785-2.
- [12] Xiaoyu Zhang, Changyuan Li, Yuting Meng, Long Yang*, and Wen Li*. Intrinsically Atomic-Disordered LuCuTe_2 as a Promising Thermoelectric Material, *ACS Appl. Energy Mater.*, 7(14):5728–5735, July 2024. doi: 10.1021/acsaem.4c00763.
- [13] Julien Lombardi, Long Yang, Nasim Farahmand, Anthony Ruffino, Ali Younes, Jonathan E. Spanier, Simon J. L. Billinge, and Stephen O’Brien. Structure and phase transitions in niobium and tantalum derived nanoscale transition metal perovskites, $\text{Ba}(\text{Ti}, \text{M}^{\text{V}})\text{O}_3$, $\text{M}=\text{Nb}, \text{Ta}$, *J. Chem. Phys. (Special Collection: Festschrift in honor of Louis E. Brus)*, 160(13):134702, April 2024. doi: 10.1063/5.0192488.
- [14] Tao Jin*, Long Yang*, Xinyue Zhang, Wen Li, and Yanzhong Pei. Close-packed layer spacing as a practical guideline for structure symmetry manipulation of IV-VI/I-V-VI₂ thermoelectrics, *InfoMat*, 6(2):e12502, February 2024. doi: 10.1002/inf2.12502.
- [15] Saman Moniri, Yao Yang, Jun Ding, Yakun Yuan, Jihan Zhou, Long Yang, Fan Zhu, Yuxuan Liao, Yonggang Yao, Liangbing Hu, Peter Ercius, and Jianwei Miao. Three-dimensional atomic structure and local chemical order of medium- and high-entropy nanoalloys, *Nature*, 624(7992):564–569, December 2023. doi: 10.1038/s41586-023-06785-z.
- [16] Yuchen Shang, Mingguang Yao, Zhaodong Liu, Rong Fu, Longbiao Yan, Long Yang, Zhongyin Zhang, Jiajun Dong, Chunguang Zhai, Xuyuan Hou, Liting Fei, GuanJie Zhang, Jianfeng Ji, Jie Zhu, He Lin, Bertil Sundqvist, and Bingbing Liu. Enhancement of short/medium-range order and thermal conductivity in ultrahard sp^3 amorphous carbon by C_{70} precursor, *Nat. Commun.*, 14(1):7860, November 2023. doi: 10.1038/s41467-023-42195-5.
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- [18] 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 *Comprehensive Inorganic Chemistry III*, pages 222–247. Elsevier, Oxford, third edition edition, January 2023.
- [19] 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.
- [20] 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.

- [21] 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, March 2021. doi: 10.1002/aelm.202001202.
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- [23] 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.
- [24] 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.
- [25] 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.
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- [28] Wei Cao, Long Yang, Stéphane Auffret, and William E. Bailey. Nearly isotropic spin-pumping related Gilbert damping in $\text{Pt}/\text{Ni}_{81}\text{Fe}_{19}/\text{Pt}$, *Phys. Rev. B*, 99(9):094406, March 2019. doi: 10.1103/PhysRevB.99.094406.
- [29] 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.
- [30] 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 $\text{Ba}(\text{Ti}_{1-x}\text{Fe}_x)\text{O}_3$ Nanocrystals, *Chem. Mater.*, 31(4):1318–1335, February 2019. doi: 10.1021/acs.chemmater.8b04447.
- [31] 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.