

Xianyuan Liu

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Research Interests

Multimodal AI, Materials Design, Drug Discovery, Computer Vision, Open-source Software

Appointments

- Academic Fellow for Multimodal AI – School of Computer Science, the University of Sheffield *from 03.2026*
- Senior AI Research Engineer – Centre for Machine Intelligence (CMI), the University of Sheffield *09.2023 – 02.2026*

Education

- PhD in Signal & Information Processing – University of Chinese Academy of Sciences, China *09.2016 – 07.2023*
- BEng in Measuring Control Technology & Instruments – Southeast University, China *09.2012 – 06.2016*

Publications [[#] indicates a supervised or co-supervised student/staff]

Journal Papers

- [J1] L. Wu, **X. Liu**, I. Palamarcu, R. Bajwa, Y. Zhang, & R. Dwyer-Joyce, “The Bearing Shell Surface Indentation and Early-state Wear Detection Combining Active Ultrasound and One-dimensional Convolutional Neural Network”, *Wear* (IF: 6.1), 591, 206592, 2026.
- [J2] **X. Liu**, J. Zhang[#], S. Zhou, T. L. van der Plas, et al., “Towards Deployment-centric Multimodal AI beyond Vision and Language”, *Nature Machine Intelligence* (IF: 23.9), 7, 1612–1624, 2025.
- [J3] P. Bai, F. Miljković, **X. Liu**, L. De Maria, R. Croasdale-Wood, O. Rackham, & H. Lu, “Mask-prior-guided Denoising Diffusion Improves Inverse Protein Folding”, *Nature Machine Intelligence* (IF: 23.9), 7, 876–888, 2025.
- [J4] X. Hao[#], **X. Liu**, Y. Liu[#], Y. Qiu, Y. Zhang, Y. Cui, & T. Lei, “Infrared Small Target Detection via Multidirectional Local Gravitational Force and Level-line Connectivity”, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing* (IF: 5.3), 18, 11111–11127, 2025.
- [J5] X. Liu, S. Rastegari, Y. Huang, S. C. Cheong, W. Liu, W. Zhao, Q. Tian, H. Wang, S. Zhou, Y. Guo, S. Tabakhi, **X. Liu**, Z. Zhu, W. Sang, & H. Lu, “Interpretable Multimodal Learning for Tumor Protein-metal Binding: Progress, Challenges, and Perspectives”, *Methods* (IF: 4.3), 242, 97–112, 2025.
- [J6] M. G. Özden, **X. Liu**, T. J. Wilkinson, M. S. Üstün-Yavuz, & N. A. Morley, “Predictive Modelling of Laser Powder Bed Fusion of Fe-based Nanocrystalline Alloys based on Experimental Data Using Multiple Linear Regression Analysis”, *Heliyon* (IF: 3.6), 10(15), e35047, 2024.
- [J7] **X. Liu**, S. Zhou, T. Lei, P. Jiang, Z. Chen, & H. Lu, “First-person Video Domain Adaptation with Multi-scene Cross-site Datasets and Attention-based Methods”, *IEEE Transactions on Circuits and Systems for Video Technology* (IF: 11.1), 33(12), 7774–7788, 2023.
- [J8] M. Lei[#], & **X. Liu**, “SOLO-Net: A Sparser but Wiser Method for Small Object Detection in Remote Sensing Images”, *IEEE Geoscience and Remote Sensing Letters* (IF: 4.4), 21, 1–5, 2023.
- [J9] Y. Liu[#], **X. Liu**, X. Hao[#], W. Tang, S. Zhang, & T. Lei, “Single-frame Infrared Small Target Detection by High Local Variance, Low-rank and Sparse Decomposition”, *IEEE Transactions on Geoscience and Remote Sensing* (IF: 8.6), 61, 1–17, 2023.
- [J10] X. Hao[#], **X. Liu**, Y. Liu[#], Y. Cui, & T. Lei, “Infrared Small-target Detection Based on Background-suppression Proximal Gradient and GPU Acceleration”, *Remote Sensing* (IF: 4.1), 15(22), 5424, 2023.
- [J11] S. Zhang, F. Song, **X. Liu**, X. Hao, Y. Liu, T. Lei, & P. Jiang, “Text Semantic Fusion Relation Graph Reasoning for Few-shot Object Detection on Remote Sensing Images”, *Remote Sensing* (IF: 4.1), 15(5), 1187, 2023.
- [J12] G. Yao, T. Lei, **X. Liu**, & P. Jiang, “Temporal Action Detection in Untrimmed Videos from Fine to Coarse Granularity”, *Applied Sciences* (IF: 2.5), 8(10), 1924, 2018.
- [J13] G. Yao, T. Lei, **X. Liu**, & P. Jiang, “Temporal Modeling on Multi-temporal-scale Spatiotemporal Atoms for Action Recognition”, *Applied Sciences* (IF: 2.5), 8(10), 1835, 2018.

Conference Papers

- [C1] J. Zhang[#], **X. Liu**, W. Wu, S. Tabakhi, W. Fan, S. Zhou, K. L. Tee, T. S. Wong, & H. Lu, “Classifying the Stoichiometry of Virus-like Particles with Interpretable Machine Learning”, in *the 47th Annual Int. Conf. of the IEEE Engineering in Medicine and Biology Society (EMBC)*, July 2025.

- [C2] H. Wang[#], **X. Liu**, A. Jungbluth, A. Ramadan, R. Oliver, & H. Lu, “Benchmarking Band Gap Prediction for Semiconductor Materials using Multimodal and Multi-fidelity Data”, in *ICLR 2025 Workshop on AI for Accelerated Materials Discovery (AI4Mat-ICLR)*, April 2025.
- [C3] M. N. I. Suvon, P. C. Tripathi, W. Fan, S. Zhou, **X. Liu**, S. Alabed, V. Osmani, A. Swift, C. Chen, & H. Lu, “Multimodal Variational Autoencoder for Low-cost Cardiac Hemodynamics Instability Detection”, in *the 27th Int. Conf. on Medical Image Computing and Computer Assisted Intervention (MICCAI, CORE A)*, pages 296–306, Oct. 2024.
- [C4] J. Wang, Z. Li, K. Sun, **X. Liu**, & Y. Zhou, “DVPE: Divided View Position Embedding for Multi-view 3D Object Detection”, in *the 33rd Int. Joint Conf. on Artificial Intelligence (IJCAI, CORE A*)*, pages 6877–6885, Aug. 2024.
- [C5] **X. Liu**, S. Zhang, T. Lei, & P. Jiang, “Cascade Attentional Fusion for Unsupervised Domain Adaptation on Multimodal Egocentric Video Analysis”, in *the 2nd Int. Conf. on Image, Signal Processing, and Pattern Recognition*, Vol. 12707, pages 135–142, June 2023.
- [C6] Q. Chen, F. Song, **X. Liu**, S. Zhang, T. Lei, & P. Jiang, “Remote Sensing Image Registration of Disaster-affected Areas based on Deep Learning Feature Matching”, in *the 2nd Int. Conf. on Digital Society and Intelligent Systems*, Vol. 12599, pages 596–604, April 2023.
- [C7] **X. Liu**, T. Lei, & P. Jiang, “Fine-grained Egocentric Action Recognition with Multi-Modal Unsupervised Domain Adaptation”, in *IEEE 6th Information Technology, Networking, Electronic and Automation Control Conf.*, Vol. 6, pages 84–90, Feb. 2023.
- [C8] H. Lu, **X. Liu**, S. Zhou, R. Turner, P. Bai, R. E. Koot, M. Chasmai, L. Schobs, & H. Xu, “PyKale: Knowledge-aware Machine Learning from Multiple Sources in Python”, in *the 31st ACM Int. Conf. on Information & Knowledge Management (CIKM, CORE A)*, pages 4274–4278, Oct. 2022.
- [C9] G. Yao, J. Zhong, T. Lei, & **X. Liu**, “Constructing Hierarchical Spatiotemporal Information for Action Recognition”, in *the 3rd Int. Conf. on Robotics, Control and Automation*, pages 596–602, Oct. 2018.
- [C10] G. Yao, **X. Liu**, & T. Lei, “Action Recognition with 3D ConvNet-GRU Architecture”, in *IEEE 15th Int. Conf. on Ubiquitous Intelligence and Computing*, pages 208–213, Aug. 2018.

Preprints

- [P1] P. Bai, **X. Liu**, W. Fan, T. Jiang, W. K. Cheung, & H. Lu, “Geometry-aware Line Graph Transformer Pre-training for Molecular Property Prediction”, *arXiv preprint arXiv:2309.00483*, 2025.
- [P2] W. Fan, M. N. I. Suvon, S. Zhou, **X. Liu**, S. Alabed, V. Osmani, A. Swift, C. Chen, & H. Lu, “MeDSLIP: Medical Dual-Stream Language-Image Pre-training for Fine-grained Alignment”, *arXiv preprint arXiv:2403.10635*, 2025.
- [P3] S. Rastegari, S. Tabakhi, **X. Liu**, W. Sang, & H. Lu, “Co-evolution-based Metal-binding Residue Prediction with Graph Neural Networks”, *arXiv preprint arXiv:2502.16189*, 2025.

Teaching

- Guest Lecturer for COM6012 Scalable Machine Learning at the University of Sheffield 2024 – 2025
- Co-supervised six MSc/MEng/BSc student dissertation projects at the University of Sheffield. *All achieved distinction*
- Co-supervised one BEng dissertation project and two junior PhD projects in China. *All led to journal publications* (with IF 4.0, 7.5, and 4.2, respectively)

Selected Talks

- “Mining the Literature: Extracting complex concentrated alloy properties with large language models”, Armourers and Brasiers’ Cambridge Forum Brief Encounters, University of Cambridge, Cambridge, June 2025.
- “Interdisciplinary AI Research for Virus-like Particle Identification and Drug Discovery”, UKSEA Vax Hub All UK Partners Meeting, the University of Sheffield, Sheffield, May 2025.
- “AI Research Engineering for Digital Materials Discovery”, Cross-Disciplinary Hydrogen Opportunities and Networking Event, the University of Sheffield, Sheffield, Mar. 2025.
- “Molecular Property Prediction”, AI in Biosciences Symposium, the University of Sheffield, Sheffield, Sept. 2024.
- “Exploring Multimodal AI beyond Vision and Language”, First Multimodal AI Research Sprint, the Alan Turing Institute, London, Nov. 2023.

Open-source Software

- Co-creator, core contributor, and maintainer of [PyKale](#), the only multimodal training library in PyTorch Landscape (450+ GitHub stars).

Professional Services

- Organiser, the Alan Turing Institute's Interest Group on Meta-Learning for Multimodal Data 2024 – Present
 - AI UK Fringe Event: the First Multimodal AI Community Forum, online, Mar. 2024
 - The Second Workshop on Multimodal AI, Sheffield, June 2024
 - The First Multimodal AI Research Sprint, London, Nov. 2023
- Organiser, Third Workshop on Multimodal AI, London, Sept. 2025
- Invited Researcher, ChemDX Hackathon, Korea Research Institute of Chemical Technology (KRICT), Seoul, South Korea, Aug. 2025
- Organiser, EMBC Workshop on “Open Biomedical Multimodal AI Research: From Pixels to Molecules”, Copenhagen, Denmark, July 2025
- Selected Journal Reviewer:
 - Nature Communications, Nature Computational Science, IEEE Transactions on Neural Networks and Learning Systems (TNNLS), IEEE Transactions on Intelligent Transportation Systems, Knowledge-Based Systems (KBS), IEEE Transactions on Cognitive and Developmental Systems (TCDS).
- Selected Conference Reviewer:
 - International Conference on Knowledge Discovery and Data Mining (SIGKDD, 2024–2026), International Conference on Medical Image Computing and Computer Assisted Intervention (MICCAI, 2025), European Conference on Artificial Intelligence (ECAI, 2024).
- Programme Reviewer:
 - European Lab for Learning & Intelligent Systems (ELLIS) PhD Programme, 2025