Xianyuan Liu

Email: xianyuan.liu@shef.ac.uk | Google Scholar: oEsfAycAAAAJ | GitHub: xianyuanliu | LinkedIn: xianyuanliu

Research Interest

AI for Materials Discovery, AI for Vaccine Manufacturing, Multimodal AI, Software Engineering, and Domain Adaptation

Present Appointment

Senior AI Research Engineer – Centre for Machine Intelligence (CMI), the University of Sheffield *Sept. 2023 – Present*

- [Research] AI for Materials Discovery (Dec. 2023 – Present)
  - Predictive modelling of laser powder bed fusion of Fe-based nanocrystalline alloys
    Outcome: A second-authored paper published in the journal *Heliyon* (IF: 3.4).
  - Extracting complex concentrated alloy properties from scientific literature with large language model (LLM)
    Outcome: A second-authored abstract accepted for an oral presentation at an international materials discovery conference in Aug. 2024
  - Discovering new sustainable magnetic materials using machine learning
  - Predicting bandgap using graph neural network and domain adaptation
- [Research] Multimodal AI Community UK Roadmap Development
  - Developing a strategy and roadmap for cross-disciplinary multimodal AI
  - Identifying cross-cutting multimodal AI challenges and potential solutions
  - Coordinating 45 researchers to draft a perspective paper on the findings, targeting *Nature Machine Intelligence*
- [Research] Machine Learning Software Library Development: PyKale
  - Co-leading code review, maintenance, and development to enhance and expand functionality and capability
  - Mentoring new developers in industry-standard software contributions, i.e. automation, testing, & documentation
- [Teaching] Guest Lecturer for COM6012 Scalable Machine Learning: 126 MSc students, 1-hour lecture, and 2-hour lab
- [Teaching] Co-supervised one MEng in Materials dissertation project (Distinction, a journal paper in preparation), General Engineering, and one MSc in Data Analytics dissertation project (ongoing), School of Computer Science
- [Service] Organiser of the Alan Turing Institute's Interest Group on Meta-Learning for Multimodal Data
  - Co-proposed and co-organised an AI UK Fringe Event: the First Multimodal AI Community Forum
  - Co-organised the Second Workshop on Multimodal AI, with 107 in-person attendees and four keynote speakers from industry, academia, and non-profit organisations, including Microsoft Research and Lloyds Banking Group
  - Co-organised the First Multimodal AI Research Sprint, with 45 selected in-person attendees from the UK and Europe
- [Leadership] Assistant Head of AI Research Engineering (AIRE)
  - Shaping strategic vision and research direction, setting objectives, and assessing progress with the Head of AIRE
  - Coordinating interdisciplinary collaborations with experts in Materials and Biological Engineering
  - Leading and managing three AI for Materials Discovery projects
  - Mentoring junior researchers and fostering a collaborative and innovative team environment
  - Recruited two AI Research Engineers, including shortlisting and conducting interviews
- [Leadership] Acting Head of AI Research Engineering (July 2024 – Aug. 2024, four weeks)
  - Leading the team aligning with the AIRE mission by overseeing project progress and managing project meetings
  - Conducting biweekly team meetings to enhance productivity, communication, and strategic alignment
  - Supervising six AI Research Engineers and providing weekly one-on-one mentorship and guidance

Previous Experience

Visiting Researcher – Department of Computer Science (DCS), the University of Sheffield *Sept. 2019 – Sept. 2021*

- [Research] Machine Learning Software Library Creation: PyKale (Mar. 2020 – Sept. 2021)
  - Co-created a Python library for accessible machine learning from multimodal data
  - Co-developed the library following FAIR principles of Findability, Accessibility, Interoperability, and Reusability
  - **Outcome:** An official member of the PyTorch ecosystem (world-leading AI framework for scientific research) and a top (CORE A) conference publication
- [Teaching] Co-supervised four student dissertation projects at DCS: one BSc in Computer Science & Mathematics, one BSc in AI & Computer Science, and two MSc in Data Analytics. *All four projects achieved distinction*.

PhD in Signal & Information Processing – University of Chinese Academy of Sciences, China *Sept. 2016 – July 2023*

- [Research] Video Domain Adaptation and Action Recognition
  - First-person video domain adaptation, including multimodal and unimodal approaches
  - EgoAction: An open video dataset for first-person video domain adaptation
  - Temporal action detection in untrimmed videos from fine to coarse granularity

  - Temporal modelling on multi-temporal-scale spatio-temporal atoms
  - Action recognition using 3D convolutional neural networks and recurrent neural networks
- [Research] Remote Sensing and Infrared Small Target Detection
  - Small object detection using attention mechanism and path aggregation network
  - Infrared small target detection using background-suppression proximal gradient and GPU acceleration
  - Single-frame infrared small target detection by high local variance, low-rank and sparse decomposition
  - Deep learning feature matching for remote sensing image registration of disaster-affected areas
- [Teaching] Supervised one BEng dissertation project and co-supervised two junior PhD projects, *all resulting in journal publications* (with IF 4.0, 7.5, and 4.2, respectively)

Grants

- Awarded
  - PI, "Learning Tensor-Based Features via 3D Convolutional Neural Network for Action Recognition", China Scholarship Council, grant total: £28,800 (Sept. 2019 – Sept. 2021).
- Grant Applications Under Review
  - Researcher Co-I (PI: Haiping Lu, Co-I: Kathy Christofidou and Nicola Morley), "LLM-Driven Data Extraction and Multimodal Graph Learning for Enhanced Materials Property Prediction", EPSRC Centre for Doctoral Training in Developing National Capability in Materials 4.0, submitted on 21st July 2024, grant total: approximately £75,000.
  - Researcher Co-I (PI: Xingyi Song, Co-I: Haiping Lu), "Large-Scale PVDF Nanofibre Performance Prediction: A Text-as-Data Approach", Royal Society, submitted on 29th May 2024, grant total: £11,420.

Research Collaborators

Internal at the University of Sheffield:

- School of Chemical, Materials and Biological Engineering:
  - Prof. Nicola Morley on material physics and functional magnetic materials
  - Prof. Kathy Christofidou on digital & sustainable metallurgy and high entropy alloys
  - Prof. Tuck Seng Wong on biomanufacturing and virus-like particle design
  - Dr Kang Lan Tee on biomanufacturing and protein engineering
  - Dr Robert Oliver on sustainable materials and solar energy
  - Dr Tom Wilkinson on sustainable construction materials and immobilisation science
- School of Computer Science:
  - Prof. Haiping Lu on machine learning and multimodal AI
  - Dr Xingyi Song on natural language processing and machine learning
  - Dr Shuo Zhou on machine learning and medical data analysis
  - Dr Donghwan Shin on software engineering and testing for AI

External:

- Mr Peizhen Bai, Senior AI Scientist at AstraZeneca, on molecular property prediction and drug discovery
- Key collaborators on multimodal AI perspective: Prof. William Cheung, Hong Kong Baptist University; Dr Nataliya Tkachenko, Lloyds Banking Group; Ms Anastasiia Grishina, University of Oslo; Prof. Honghan Wu, University of Glasgow; Prof. Greg Slabaugh, Queen Mary University of London; Dr Ben Evans, British Antarctic Survey; Dr Dan Schofield, NHS England; Dr Peter Charlton, University of Cambridge; Dr Tingting Zhu, University of Oxford; Dr Thijs van der Plas, the Alan Turing Institute.

Selected Talks

- "Dual-modality Graph Transformer Pre-training for Molecular Property Prediction", AI in Biosciences Symposium, the University of Sheffield, Sheffield, scheduled in Sept. 2024.
- "Multimodal AI for Engineering", First Multimodal AI Community Forum, AI UK Fringe Event, Online, Mar. 2024.
- "Digital Materials Discovery", Shef.AI Community Meeting 7, the University of Sheffield, Sheffield, Mar. 2024.
- "Exploring Multimodal AI beyond Vision and Language", First Multimodal AI Research Sprint, the Alan Turing Institute, London, Nov. 2023.

Academic Services

- Journal Reviewer:
  - IEEE Transactions on Neural Networks and Learning Systems (IF: 10.2)
  - IEEE Transactions on Cognitive and Developmental Systems (IF: 5)
  - IEEE Sensors Journal (IF: 4.3)
  - The Visual Computer (IF: 3)
  - BMC Bioinformatics (IF: 2.9)
  - Earth Science Informatics (IF: 2.7)

- Conference Reviewer:
  - International Conference on Knowledge Discovery and Data Mining (SIGKDD, CORE A*), 2024
  - British Machine Vision Conference (BMVC, CORE A), 2021

Publications

Journal Papers [# indicates supervised or co-supervised students]

[J1] [Materials Discovery] Özden, M. G., **Liu, X.**, Wilkinson, T. J., Üstün-Yavuz M. S., & Morley, N. A. (2024). Predictive Modelling of Laser Powder Bed Fusion of Fe-based Nanocrystalline Alloys based on Experimental Data using Multiple Linear Regression Analysis. *Heliyon (IF: 3.4)*.

[J2] [Computer Vision] **Liu, X.**, Zhou, S., Lei, T., Jiang, P., Chen, Z., & Lu, H. (2023). 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: 8.3)*, 33(12), 7774-7788.

[J3] [Remote Sensing] Lei, M.#, & **Liu, X.** (2023). SOLO-Net: A Sparser but Wiser Method for Small Object Detection in Remote Sensing Images. *IEEE Geoscience and Remote Sensing Letters (IF: 4.0)*, 21, 1-5.

[J4] [Remote Sensing] Liu, Y.#, **Liu, X.**, Hao, X., Tang, W., Zhang, S., & Lei, T. (2023). Single-frame Infrared Small Target Detection by High Local Variance, Low-rank and Sparse Decomposition. *IEEE Transactions on Geoscience and Remote Sensing (IF: 7.5)*, 61, 1-17.

[J5] [Remote Sensing] Hao, X.#, **Liu, X.**, Liu, Y., Cui, Y., & Lei, T. (2023). Infrared Small-Target Detection Based on Background-Suppression Proximal Gradient and GPU Acceleration. *Remote Sensing (IF: 4.2)*, 15(22), 5424.

[J6] [Remote Sensing] Zhang, S., Song, F., **Liu, X.**, Hao, X., Liu, Y., Lei, T., & Jiang, P. (2023). Text Semantic Fusion Relation Graph Reasoning for Few-shot Object Detection on Remote Sensing Images. *Remote Sensing (IF: 4.2)*, 15(5), 1187.

[J7] [Computer Vision] Yao, G., Lei, T., **Liu, X.**, & Jiang, P. (2018). Temporal Action Detection in Untrimmed Videos from Fine to Coarse Granularity. *Applied Sciences (IF: 2.5)*, 8(10), 1924.

[J8] [Computer Vision] Yao, G., Lei, T., **Liu, X.**, & Jiang, P. (2018). Temporal Modeling on Multi-temporal-scale Spatiotemporal Atoms for Action Recognition. *Applied Sciences (IF: 2.5)*, 8(10), 1835.

Conference Papers

[C1] [Computer Vision] Wang, J., Li, Z., Sun, K. **Liu, X.** & Zhou, Y. (2024, Aug.). DVPE: Divided View Position Embedding for Multi-View 3D Object Detection. In *the 33rd Int. Joint Conf. on Artificial Intelligence (**IJCAI, CORE A***)*.

[C2] [Medical Imaging] Suvon, M. N. I., Tripathi, P. C., Fan, W., Zhou, S., **Liu, X.**, Alabed, S., Osmani, V., Swift, A., Chen, C., & Lu, H. (2024, Oct.). 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**)*.

[C3] [Computer Vision] **Liu, X.**, Zhang, S., Lei, T., & Jiang, P. (2023, June). Cascade Attentional Fusion for Unsupervised Domain Adaptation on Multi-modal Egocentric Video Analysis. In *the 2nd Int. Conf. on Image, Signal Processing, and Pattern Recognition* (Vol. 12707, pp. 135-142).

[C4] [Remote Sensing] Chen, Q., Song, F., **Liu, X.**, Zhang, S., Lei, T., & Jiang, P. (2023, April). 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, pp. 596-604).

[C5] [Computer Vision] **Liu, X.**, Lei, T., & Jiang, P. (2023, Feb.). Fine-grained Egocentric Action Recognition with Multi-Modal Unsupervised Domain Adaptation. In *IEEE 6th Information Technology, Networking, Electronic and Automation Control Conf.* (Vol. 6, pp. 84-90).

[C6] [Software Engineering] Lu, H., **Liu, X.**, Zhou, S., Turner, R., Bai, P., Koot, R. E., Chasmai, M., Schobs, L., & Xu, H. (2022, Oct.). PyKale: Knowledge-aware Machine Learning from Multiple Sources in Python. In *the 31st ACM Int. Conf. on Information & Knowledge Management (**CIKM, CORE A**)* (pp. 4274-4278).

[C7] [Computer Vision] Yao, G., Zhong, J., Lei, T., & **Liu, X**. (2018, Oct.). Constructing Hierarchical Spatiotemporal Information for Action Recognition. In *the 3rd Int. Conf. on Robotics, Control and Automation* (pp. 596-602).

[C8] [Computer Vision] Yao, G., **Liu, X.**, & Lei, T. (2018, Aug.). Action Recognition with 3D ConvNet-GRU Architecture. In *IEEE 15th Int. Conf. on Ubiquitous Intelligence and Computing* (pp. 208-213).

Abstract

[A1] [Materials Discovery] Thomas, A.#, **Liu, X.**, Berry, J., Wilkinson, T., Lu, H., Morley, N. A., & Christofidou, K. A. (2024, Aug.). Extracting Complex Concentrated Alloys Properties from Scientific Literature with LLMs. *Accelerate Conference* (oral presentation).

Preprints

[P1] [Biomaterials] Bai, P., **Liu, X.**, & Lu, H. (2023). Geometry-aware Line Graph Transformer Pre-training for Molecular Property Prediction. *arXiv preprint arXiv:2309.00483*.

[P2] [Medical Imaging] Fan, W., Suvon, M. N. I., Zhou, S., **Liu, X.**, Alabed, S., Osmani, V., Swift, A., Chen, C., & Lu, H. (2024). MeDSLIP: Medical Dual-Stream Language-Image Pre-training for Fine-grained Alignment. *arXiv preprint arXiv:2403.10635*.