

Mingxiao Li

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WORKING EXPERIENCE

Shanghai AI Laboratory, AI for Science Center

Shanghai, China

Young Researcher

Dec. 2025 – Present

- Research Interests: Molecular Generation, Unified Molecular Tokenization, and Reasoning Models for Bioscience

KU Leuven

Leuven, Belgium

Postdoctoral Researcher in Computer Science

Nov. 2024 - Jun. 2025

- Advisor: Prof. Marie-Francine Moens
- Research Interests: Visual Generative Models, Story Generation, Multimodal Large Language Models

EDUCATION

KU Leuven

Leuven, Belgium

Ph.D. in Computer Science

Sept. 2019 - Nov. 2024

- Advisor: Prof. Marie-Francine Moens
- Thesis: Leveraging External Knowledge in Deep Learning and Conditional Generative Models.
- **Awarded summa cum laude with the congratulations of the examination committee (greatest distinction), ranked in the top 5% of the Faculty of Engineering Science.**

KU Leuven

Leuven, Belgium

Master of Artificial Intelligence

Sept. 2018 - Sept. 2019

KU Leuven

Leuven, Belgium

Master of Theoretical Chemistry and Computational Modeling

Sept. 2016 - Jun. 2018

East China University of Science and Technology

Shanghai, China

Bachelor of Material Physics

Sept. 2011 - Jun. 2015

- *Academic scholarship*: Academic year 2011-2012, 2012-2013, 2013-2014, 2014-2015
- *Honors Graduate*: (Top 5% students in Department of Material)

RESEARCH FOCUS

AI for Science. My current research at Shanghai AI Laboratory focuses on molecular generation, unified molecular tokenization, and reasoning models for bioscience. I am particularly interested in generative foundation models for scientific discovery.

Diffusion Models and Video Generation. My previous work investigated sampling algorithms for diffusion models, including shifted diffusion time steps to mitigate exposure bias. I also explored controllable image-to-video generation driven by user-specified object motion.

Large Language and Multimodal Models. I have explored long-form video understanding with large language models and am interested in extending LLMs and multimodal large language models toward scientific reasoning.

SELECTED PUBLICATIONS

- **Mingxiao Li**, Ning Mang, Marie-Francine Moens. Consistent Story Generation: Unlocking the Potential of Zigzag Sampling. *Advances on Neural Information Processing Systems. (NeurIPS 2025)* .[Paper] [Code]
- **Mingxiao Li***, Bo Wan*, Marie-Francine Moens & Tinne Tuytelaars. Animate Your Motion: Turning Still Images into Dynamic Videos. *European Conference on Computer Vision (ECCV 2024)* .[Paper] [Code]
- **Mingxiao Li***, Tingyu Qu*, Ruicong Yao, Wei Sun, & Marie-Francine Moens. Alleviating Exposure Bias in Diffusion Models through Sampling with Shifted Time Steps. *International Conference on Learning Representations (ICLR 2024)*. [Paper] [Code (DDPM ver.)][Code (ADM ver.)]

- Mang Ning, **Mingxiao Li ***, Jianlin Su *, Haozhe Jia, Lanmiao Liu, Martin Beneš, Albert Ali Salah, Itir Onal Ertugrul. DCTdiff: Intriguing Properties of Image Generative Modeling in the DCT Space. *International Conference on Machine Learning (ICML 2025)*. [Paper] [Code]
- Mang Ning, **Mingxiao Li**, Jianlin Su, Albert Ali Salah & Itir Onal Ertugrul. Elucidating the Exposure Bias in Diffusion Models. *International Conference on Learning Representations (ICLR 2024)*. [Paper] [Code]
- Jingyuan Sun*, **Mingxiao Li***, Zijiao Chen, Yunhan Zhang, Shaonan Wang, & Marie-Francine Moens. Contrast, Attend and Diffuse to Decode High-Resolution Images from Brain Activities. *Advances on Neural Information Processing Systems. (NeurIPS 2023)*. [Paper] [Code]
- **Mingxiao Li***, Zehao Wang*, Tinne Tuytelaars, & Marie-Francine Moens. Layout-Aware Dreamer for Embodied Visual Referring Expression Grounding. *Proceedings of the AAAI Conference on Artificial Intelligence (AAAI 2023)* (**Oral Presentation**). [Paper] [Code]
- **Mingxiao Li**, Marie-Francine Moens. Dynamic Key-value Memory Enhanced Multi-step Graph Reasoning for Knowledge-based Visual Question Answering. *Proceedings of the AAAI Conference on Artificial Intelligence (AAAI 2022)*. [Paper][Code]
- Jingyuan Sun*, **Mingxiao Li***, Zijiao Chen, Marie-Francine Moens. NeuroCine: Decoding Vivid Video Sequences from Human Brain Activities. *Proceedings of the AAAI Conference on Artificial Intelligence (AAAI 2025)* (**Oral Presentation**). [Paper]

SELECTED PREPRINTS

- Tingyu Qu, **Mingxiao Li**, Tinne Tuytelaars, Marie-Francine Moens. TS-LLaVA: Constructing Visual Tokens through Thumbnail-and-Sampling for Training-Free Video Large Language Models [Paper][Code]
- Maria Mihaela Trusca, **Mingxiao Li**, Marie-Francine Moens. Action-based image editing guided by human instructions. [Paper]

* denotes equal contribution

AWARD

KU Leuven PhD graduate with summa cum laude (highest distinction), ranked in the top 5% of the Faculty of Engineering Science (2024)

European Union Erasmus Mundus Full Scholarship. (2016-2018)

Chinese Government Scholarship for Outstanding Undergraduate Students. (2015)

SERVICES

Reviewer: ICML, CVPR, ICLR, NeurIPS, EMNLP, ACL, AAAI, EACL, ECML, ECAI

Area Chair: ACL Rolling Review (2025.02)

Workshop Organizer: AAAI-2024 Workshop: Artificial Intelligence for Brain Encoding and Decoding (AIBED)