Lanqing Li

lanqingli1993@gmail.com | +86 18171192701 | Shenzhen, China, 518102

Personal Profile

- I'm a final-year PhD in computer science and engineering at The Chinese University of Hong Kong with 7+ years of experience in industrial research labs, undertaking principal investigator at Zhejiang Lab (2023-2026), and senior research scientist (T10) at Tencent AI Lab (2019-2023) working on machine learning and its applications in drug discovery and autonomous control. Prior to my endeavor in AI research, I received training in physics from MIT and UChicago, and was also a gold medalist of the International Physics Olympiad (IPHO 2011), winning the Prize of Best Score in Theory.
- **Homepage**: https://lanqingli1993.github.io/
- **Research Interests**: Machine Learning, AI for Science (AI4Sci), Reinforcement Learning (RL), AI for Drug Discovery (AIDD).
- **Research Highlights**: As a machine learning researcher, I pioneered a novel paradigm called offline meta-RL (OMRL) for pre-training generalist decision-making models and AI agents, by proposing the first model-free OMRL algorithm FOCAL. Subsequently, I developed an information-theoretic framework called UNICORN to unify existing methods in the field, paving the way to a general pre-training paradigm of foundation models for decision making. As an AI4Sci researcher, I led the first AI-driven large-scale screening of human proteome, revealing 12/15 novel materials for gene packaging and delivery *in vitro*, with implications for next-generation gene therapy and programmable nanomedicine.
- **Expected Graduation Date**: Dec, 2026

Employment History

Zhejiang Lab **(more info)** *Hangzhou, China*

Principal Investigator, Research Center for Life Sciences Computing *01/2023-01/2026*

- Led the R&D of several core AIDD projects:
  1. Protein design and engineering for mRNA delivery
  2. Biocatalysis modeling and enzyme engineering.
  3. AI agent for drug discovery
- Successfully concluded and defended a 20-million-yuan research project on "Digital Cell and Intelligent Computing Platform".
- Mentor of 4 employees and 10+ Ph.D. students.

Tencent *Shenzhen, China*

Senior Research Scientist, AI Lab *10/2019-01/2023*

- Co-developed the multi-step retrosynthesis module of iDrug. Independently developed a state-of-the-art model for synthetic accessibility prediction, in collaboration with the American Chemical Society (CAS).
- Led the research and development of the core AI algorithms and greenhouse simulator of the iGrow solution, in collaboration with Wageningen University & Research (WUR).
- Co-PI of the Tencent AI Lab Rhino-Bird Elite Training Program and Tencent AI Lab Rhino-Bird Focused Research Program, with a focus on robust learning and retrosynthesis.
- Mentor of 1 employee and 15+ research interns at the machine learning center.

Academic History

The Chinese University of Hong Kong *08/2022-Now*

Ph.D. Candidate in Computer Science and Engineering

- Supervisor: Prof. Pheng Ann Heng

- Research area: Robust Learning, AI for Science

The University of Chicago *09/2015-2017/08*

Master of Science (Ph.D. Program) in Physics

Massachusetts Institute of Technology *08/2012-06/2015*

Bachelor of Science in Physics *Major GPA: 4.7/5.0*

- Research Advisor: Prof. Alan Guth, Prof. David Kaiser
- Academic Advisor: Prof. Nevin Weinberg.
- Concentration: Theoretical Cosmology, High Energy Physics

Imperial College London *06/2014-08/2014*

Summer Research Exchange Student (2 awardees from MIT Department of Physics)

- Advisor: Prof. Amihay Hanany

Peking University *09/2011-06/2012*

Candidate for a Bachelor of Science in Physics *Major GPA: 3.88/4.0*

Selected Publications (*: co-first author, †: corresponding author) (Full List)

- **Articles in Peer-Reviewed Journals**
  1. **Li, L.***, Huang, Y.*, Qian, W., Yu, J., Zhao, H., Wang, X., Zhang, O., Chen, G., Gu, S., Heng, P., Hou, T., Kang, Y. Accurate and Task-Agnostic Modeling of Enzymatic Reactions through Multimodal Relational Learning. Accepted by **Acta Pharmaceutica Sinica B (JCR Q1, IF 14.7)**.
  2. Wang, B., Li, J., Zhou, D., **Li, L.**, Li, J., Wang, E., Hao, J., Shi, L., Lu, C., Qiu, J., Hou, T., Cao, D., Chen, G., Heng, P. Unified and Explainable Molecular Representation Learning for Imperfectly Annotated Data from the Hypergraph View. **Nature Communications** 16, (2025): 8717.
  3. Gao, Z., Jiang, C., Zhang, J., Jiang, X., **Li, L.**, Zhao, P., Yang, H., Huang, Y., Li, J. Hierarchical graph learning for protein–protein interaction. **Nature Communications** 14.1 (2023): 1093.
- **Articles in Peer-Reviewed Conference Proceedings**
  1. Zhang, H., Zheng, B., Ji, T., Liu, J., Guo, A., Zhao, J., **Li, L.**†. Scrutinize What We Ignore: Reining In Task Representation Shift Of Context-Based Offline Meta Reinforcement Learning. **ICLR 2025.**
  2. **Li, L.***, Zhang, H.*, Zhang, X., Zhu, S., Yu, Y., Zhao, J., Heng, P. Towards an Information Theoretic Framework of Context-based Offline Meta-Reinforcement Learning. **NeurIPS 2024 Spotlight, Top 2.47% (387/15671), Top 0.2% (33/15671) in review score**.
  3. **Li, L.***, Zhou, Z.*, Zhao, P., Heng, P., Gong, W. Class-Conditional Sharpness-Aware Minimization for Deep Long-Tailed Recognition. **CVPR 2023.**
  4. Wang, D., **Li, L.**†, Zhao, P., Heng, P., Zhang, M. On the Pitfall of Mixup Training for Uncertainty Calibration. **CVPR 2023.**
  5. Zeng, L., **Li, L.**†, Gao, Z., Zhao, P., Li, J. ImGCL: Revisiting Graph Contrastive Learning on Imbalanced Node Classification. **AAAI 2023.**
  6. Gao, Z., Niu, Y., Cheng, J., Tang, J., Xu, T., Zhao, P., **Li, L.**†, Tsung, F., Li, J. Handling Missing Data via Max-Entropy Regularized Graph Autoencoder. **AAAI 2023.**
  7. Liu, S., Ying, R., Dong, H., **Li, L.**†, Xu, T., Rong, Y., Zhao, P., Huang, J., Wu, D. Local Augmentation for Graph Neural Networks. **ICML 2022.**
  8. **Li, L.**, Yang, R., Luo, D. FOCAL: Efficient Fully-Offline Meta-Reinforcement Learning via Distance Metric Learning and Behavior Regularization. **ICLR 2021.**
- **In Submission to Journals and Conferences**
  1. **Li, L.***†, Xun, D.*, Liu, Y., Yang, Z., Liang, Q., Zou, J., Li, K., Zhu, Z., Zhang, J., Lang, L., Liu, K., Wang, X., Tian, M., Chen, G., An, B., Heng, P., Zhong, C. AI-Driven Discovery and Engineering of Human Endogenous Nanocage Proteins for mRNA Delivery. Under external review at **Nature**

Communications.

2. **Li, L.***, Zeng, L.*, Gao, Z., Yuan, S., Bian, Y., Wu, B., Zhou, Z., Xu, H., Li, J., Zhao, P., Heng, P. Benchmarking Imbalanced Learning for AI-Aided Drug Discovery. Under major revision at **Nature Communications.**

Selected Awards and Honors

Global Young Scientists Summit - Finalist	*2025*
Prize for Best Poster, Interdisciplinary Forum of Synthetic Biology	*2025*
Prize for Research Excellence, Zhejiang Lab	*2024*
NSFC Young Scientists Fund	*2024*
Prize for Sustainable Social Values, Tencent	*2021*
SAIL Award at World Artificial Intelligence Conference - Finalist	*2020*
Distinguished Sachs Fellowship, UChicago	*2015*
Li & Fung Scholarship, MIT	*2014*
Jay Tsun Shaw (1946) Memorial Scholarship, MIT	*2013-2015*
First Prize in Young Physicists Tournaments, Peking University	*2012*
Mingde Scholarship, Peking University	*2011*
Excellent Student Scholarship, Peking University	*2011*
Gold Medalist of International Physics Olympiad	*2011*

- *Ranked 1st in Theory and 5th in Total Score*
- *Prize of Best Score in Theory (Full Marks)*

Academic Activities

- **Invited Talks and Seminars**
  1. *Trustworthy AI and Applications For Scientific (Biomedical) Discovery*, Shanghai Jiao Tong University, invited by Prof. Peilin Zhao. (12/2025)
  2. *Pre-training paradigm of foundation models for decision making*, Shanghai Jiao Tong University, invited by Prof. Peilin Zhao. (07/2025)
  3. *AI Agent: Principles and Applications*, 1st speaker at CAAI Embodied AI Youth Symposium, invited by Prof. Junqiao Zhao. (12/2023)
  4. *Intelligent Drug Discovery Platform and Its Applications*, presented at the "Computation + Biology" Youth Academic Research Symposium, Zhejiang lab. (09/2023)
  5. *Guest lecture on reinforcement learning applications*, The Chinese University of Hong Kong, Shenzhen, invited by Prof. Baoxiang Wang. (02/2023)
- **Services**
  - NSFC Grant Reviewer
  - Reviewer, TPAMI
  - Program Comittee Member, ICLR 2024-now
  - Program Comittee Member, CVPR 2023-now
  - Program Comittee Member, ICML 2022-now
  - Program Comittee Member, NeurIPS 2022-now
  - Program Comittee Member, IJCAI 2021-2022
- **Teaching and Mentoring**
  1. TA of PHYS 130 Series, UChicago *09/2016-06/2017*
  2. TA of PHYS 14200 Honors Electricity & Magnetism, UChicago *01/2016-03/2016*
  3. TA of PHYS 14100 Honors Mechanics, UChicago *09/2015-12/2015*
  4. PRIMES Circle Mentor, MIT Department of Mathematics *02/2014-12/2014*

- **Science Outreach**
  - *Modeling Biological World with Intelligent Computing*, interview by Zhejiang Lab. (11/2023)
  - *Artificial Protein Design with Inverse Folding Models*, interview by CCTV-3. (09/2023)

Referees (prioritized)

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1. **Prof. Pheng-Ann Heng**
   Choh-Ming Li Professor of Computer Science and Engineering/Director of the Institute of Medical Intelligence and XR
   The Chinese University of Hong Kong
   Email: pheng@cse.cuhk.edu.hk

2. **Prof. Chao Zhong**
   Professor/Center Director of Materials Synthetic Biology Center (MSBC)/Assistant of iSynBio Director, Institute of Synthetic Biology
   Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences
   Email: chao.zhong@siat.ac.cn

3. **Prof. Peilin Zhao**
   Professor at School of Artificial Intelligence
   Shanghai Jiao Tong University
   Email: peilinzhao@sjtu.edu.cn

4. **Prof. Junzhou Huang, FAIMBE**
   Jenkins Garrett Professor
   Department of Computer Science and Engineering
   The University of Texas at Arlington
   Email: jzhuang@uta.edu

5. **Prof. Guangyong Chen**
   Professor and Associate Director, Center for Medical AI
   Hangzhou Institute of Medicine, Chinese Academy of Sciences
   Email: chenguangyong@him.cas.cn