

# Lanqing Li

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## Personal Profile

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- I'm a principal investigator at [Zhejiang Lab](#) starting from Jan 2023, leading the computational genomics group at the Research Center for Computational Life Sciences. Previously I was a senior research scientist (T10) at [Tencent AI Lab](#), working on machine learning and its applications in drug discovery and autonomous control. I also worked as a tech lead at [InferVision](#), a pre-IPO medical AI startup.
- **Homepage:** <https://lanqingli1993.github.io/>
- **Research Interests:** Machine Learning, Reinforcement Learning (RL), AI for Drug Discovery (AIDD), AI for Science.
- **Research Highlights:** As a machine learning researcher, I pioneered a new learning paradigm called offline meta-RL (OMRL) for pre-training powerful decision-making models and AI agents, by inventing the first model-free OMRL algorithm [FOCAL](#). I subsequently proposed a theoretical framework called [UNICORN](#) to unify existing works in the field, providing principled guidelines for future research.

## Employment History

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- Zhejiang Lab* *Hangzhou, China*  
**Principal Investigator, Research Center for Life Sciences Computing** *01/2023-Now*
- R&D of RL-based and LLM-based AI agent for drug discovery and biomolecular design.
  - Leading several core AIDD projects:
    1. Design of virus-like particle (VLP)-based delivery system.
    2. Synthesis planning and biocatalysis modeling.
    3. mRNA vaccine and sequence design.
  - Mentor of 4 employees and 10+ Ph.D. students.
- Shenzhen Tencent Computer System Co., Ltd.* *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-mentored the [Tencent AI Lab Rhino-Bird Elite Training Program](#) and [Tencent AI Lab Rhino-Bird Focused Research Program](#), with focuses on robust learning and retrosynthesis.
  - Mentor of 1 employee and 20+ interns at the machine learning center.
- InferVision Medical Technology Co., Ltd.* *Beijing, China*  
**Tech Lead & Machine Learning Engineer** *03/2018-10/2019*
- Led a team of 8 engineers to develop computer-aided detection (CAD) solutions like InferRead Mammo Breat and InferRead CT Coronary.

## Academic History

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- 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*

- Concentration: Theoretical Biophysics & Computer Vision

**Massachusetts Institute of Technology**

08/2012-06/2015

*Bachelor of Science in Physics*

Major GPA: 4.7/5.0

- Advised by [Prof. Alan Guth](#), [Prof. David Kaiser](#) and [Prof. Nevin Weinberg](#).

- Concentration: Theoretical Cosmology, High Energy Physics

**Imperial College London**

06/2014-08/2014

*Exchange Student of Summer Research Placement*

**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)**

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- **Articles in Peer-Reviewed Journals**

1. Ma, K., Yang, H., Yang, S., Zhao, K., **Li, L.**, Chen, Y., Huang, J., Cheng, J., Rong, Y. "Solving the non-submodular network collapse problems via Decision Transformer." *Neural Networks* (2024): 106328.
2. Liu, Z., Liu, L., Wu, B., **Li, L.**, Wang, X., Yuan, B., Zhao, P. [Dynamics Adapted Imitation Learning](#). *Transactions on Machine Learning Research* (2023).
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. **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**.
2. Zhou, Z.\*, **Li, L.\***, Zhao, P., Heng, P., Gong, W. Class-Conditional Sharpness-Aware Minimization for Deep Long-Tailed Recognition. CVPR 2023.
3. Wang, D., **Li, L.†**, Zhao, P., Heng, P., Zhang, M. On the Pitfall of Mixup Training for Uncertainty Calibration. CVPR 2023.
4. Zeng, L., **Li, L.†**, Gao, Z., Zhao, P., Li, J. ImGCL: Revisiting Graph Contrastive Learning on Imbalanced Node Classification. AAAI 2023.
5. 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.
6. 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.
7. **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.\***, 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 by Nature Communications.
2. Huang, Y.\*, **Li, L.\***, Qian, W., Yu, J., Zhao, H., Zhang, O., Chen, G., Gu, S., Heng, P., Hou, T., Kang, Y. ERAM: A Unified Dual-Grained Cross-Modal Molecular Representation Learning Framework for Enzymatic Reaction. Under review by Advanced Science.
3. 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. Under review by ICLR 2025. (current scores: 6, 6, 8, 8)

**Selected Awards**

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Prize of 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
• <i>Ranked 1st in Theory and 5th in Total Score</i>	
• <i>Prize of Best Score in Theory (Full Marks)</i>	

## Academic Activities

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### • Invited Talks and Seminars

1. *AI Agent: Principles and Applications*, 1st speaker at CAAI Embodied AI Youth Symposium, invited by [Prof. Junqiao Zhao](#). (12/2023)
2. *Intelligent Drug Discovery Platform and Its Applications*, presented at the "Computation + Biology" Youth Academic Research Symposium, Zhejiang lab. (09/2023)
3. *Guest lecture on reinforcement learning applications*, The Chinese University of Hong Kong, Shenzhen, invited by [Prof. Baoxiang Wang](#). (02/2023)

### • Services

- Area Chair, ICML 2025
- Reviewer, TPAMI
- Reviewer, ICLR 2024
- Reviewer, CVPR 2023
- Reviewer, ICML 2022, 2023
- Reviewer, NeurIPS 2022, 2023
- Reviewer, 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)