

Lanqing Li

lanqingli1993@gmail.com | +86 18171192701 | Hangzhou, China, 311121

Personal Profile

- I'm a principal investigator at [Zhejiang Lab](#) starting from Jan 2023, leading the molecular design & synthesis group at the Center for Computational Drug Discovery. 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/Deep Learning, AI-Aided Drug Discovery (AIDD), Robust Machine Learning, Reinforcement Learning, AI for Science.

Employment History

Zhejiang Lab

Hangzhou, China

Principal Investigator, Center for Computational Drug Discovery

01/2023-Now

- Leading the research and development of state-of-the-art AI algorithms for drug design and synthesis.

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-mentoring the [Tencent AI Lab Rhino-Bird Elite Training Program](#) and [Tencent AI Lab Rhino-Bird Focused Research Program](#), covering topics on deep graph learning, OOD/Long-tailed learning, retrosynthesis, graph generation for molecular de novo design and reinforcement learning.
- Submitted 20+ research papers and patent applications, 13 of which have been published at top conferences/journals.
- 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 Breast and InferRead CT Coronary.

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 areas: AI for Drug Discovery, Robust Machine Learning, Reinforcement Learning

The University of Chicago

09/2015-08/2017

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

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

• Articles in Peer-Reviewed Journals

1. 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.
2. Zhu, S., Bai, Q., **Li, L.**, Xu, T. *Drug repositioning in drug discovery of T2DM and repositioning potential of antidiabetic agents*. Computational and Structural Biotechnology Journal (2022).
3. Hertzberg, M. P., Karouby, J., Spitzer, W. G., Becerra, J. C., & **Li, L.** *A Theory of Self-Resonance After Inflation, Part 1: Adiabatic and Isocurvature Goldstone Modes*. Phys. Rev. D 90, 123528 (2014).
4. Hertzberg, M. P., Karouby, J., Spitzer, W. G., Becerra, J. C., & **Li, L.** *A Theory of Self-Resonance After Inflation, Part 2: Quantum Mechanics and Particle-Antiparticle Asymmetry*. Phys. Rev. D 90, 123529 (2014).

• Articles in Peer-Reviewed Conference Proceedings

1. Zhou, Z.*, **Li, L.***, Zhao, P., Heng, P., Gong, W. Class-Conditional Sharpness-Aware Minimization for Deep Long-Tailed Recognition. CVPR 2023.
2. Wang, D., **Li, L.†**, Zhao, P., Heng, P., Zhang, M. On the Pitfall of Mixup Training for Uncertainty Calibration. CVPR 2023.
3. Zeng, L., **Li, L.†**, Gao, Z., Zhao, P., Li, J. ImGCL: Revisiting Graph Contrastive Learning on Imbalanced Node Classification. AAAI 2023.
4. 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.
5. Ji, Y., Zhang, L., Wu, J., Wu, B., **Li, L.**, et al. DrugOOD: Out-of-Distribution Dataset Curator and Benchmark for AI-aided Drug Discovery – A Focus on Affinity Prediction Problems with Noise. AAAI 2023.
6. Han, Z., Liang, Z., Yang, F., Liu L., **Li, L.**, et al. *UMIX: Improving Importance Weighting for Subpopulation Shift via Uncertainty-Aware Mixup*. NeurIPS 2022.
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. Gao, C., Xu, K., Zhou, K., **Li, L.**, et al. *Value Penalized Q-Learning for Recommender Systems*. SIGIR 2022.
9. Cao, X., Yao Y., **Li, L.**, et al. *iGrow: A Smart Agriculture Solution to Autonomous Greenhouse Control*. AAAI 2022.
10. **Li, L.**, Yang, R., Luo, D. *FOCAL: Efficient Fully-Offline Meta-Reinforcement Learning via Distance Metric Learning and Behavior Regularization*. ICLR 2021.
11. An, Z., Cao, X., Yao, Y., Zhang, W., **Li, L.**, Wang, Y., Guo, S., and Luo, D. *A Simulator-based Planning Framework for Optimizing Autonomous Greenhouse Control Strategy*. ICAPS 2021.

Selected Awards

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>	

Scientific Community Activities

- **Invited Talks and Seminars**

- The Chinese University of Hong Kong, Shenzhen. Guest lecture on reinforcement learning applications, invited by Prof. Baoxiang Wang. (02/2023)

- **Academic Services**

- Reviewer, TPAMI
- Reviewer, CVPR 2023
- Reviewer, NeurIPS 2022
- Reviewer, ICML 2022, 2023
- Reviewer, IJCAI 2021, 2022