Lanqing Li

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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 *1/2023-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 *10/2019-1/2023*

- 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

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)

- **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*

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

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