Lanqing Li

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Personal Profile

- I'm an incoming postdoctoral scholar at Stanford Medicine with 8+ years of experience in industrial research labs and AI startups, 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 built DeepDelievery, the first AI-driven platform to discover human-derived proteins for mRNA delivery, revealing 12/15 novel materials for gene packaging and delivery *in vitro*, with implications for next-generation gene therapy and programmable nanomedicine. My recent work aims to advance biological foundation models through the development of principled and translational alignment algorithms, proposing the first label-free post-training method for protein language models, with manuscript featured by BiologyAIDaily and DailyPapers.

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 secured 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.

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 such as InferRead Mammo Breast and InferRead CT Coronary.

Academic History

Stanford University *09/2026-now*

Postdoctoral Scholar in Bioengineering

- Supervisor: Prof. Le Cong, Prof. Mengdi Wang (Princeton)
- Research Focus: AI for Biology

The Chinese University of Hong Kong (CUHK) *08/2022-07/2026*

Ph.D. in Computer Science and Engineering

- Supervisor: Prof. Pheng Ann Heng
- Thesis: Trustworthy Representation Learning: Fairness, Faithfulness, and Alignment for Deep Learning and Biomolecular Discovery

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 publications at Google Scholar: https://scholar.google.com/citations?user=n8IjgKkAAAAJhl=en

- **Articles in Peer-Reviewed Journals**
  1. **AI-Driven Discovery and Engineering of Human-Derived Protein Scaffolds for mRNA Delivery**
     Dongmin Xun*, **Lanqing Li***†, Jie Zou*, Yi Liu, Ziyue Yang, Qianyi Liang, Ke Li, Zhu Zhu, Jicong Zhang, Lijun Lang, Kun Liu, Xinyu Wang, Meilin Tian, Guangyong Chen, Jun Yang, Bolin An, Pheng Ann Heng, Chao Zhong
     Nature Communications 2026
  2. **Accurate and Task-Agnostic Modeling of Enzymatic Reactions through Multimodal Relational Learning**
     Yuansheng Huang*, **Lanqing Li***, Wenjia Qian, Jiahui Yu, Huifeng Zhao, Xiaorui Wang, Odin Zhang, Guangyong Chen, Shukai Gu, Pheng-Ann Heng, Tingjun Hou, Yu Kang
     Acta Pharmaceutica Sinica B 2026 Editor's Highlight
  3. **Unified and Explainable Molecular Representation Learning for Imperfectly Annotated Data from the Hypergraph View**
     Bowen Wang, Junyou Li, Donghao Zhou, **Lanqing Li**, Jinpeng Li, Ercheng Wang, Jianye Hao, Liang Shi, Chengqiang Lu, Jiezhong Qiu, Tingjun Hou, Dongsheng Cao, Guangyong Chen, Pheng Ann Heng
     Nature Communications 2025
  4. **Hierarchical Graph Learning for Protein–Protein Interaction**
     Ziqi Gao, Chenran Jiang, Jiawen Zhang, Xiaosen Jiang, **Lanqing Li**, Peilin Zhao, Huanming Yang, Yong Huang Jia Li
     Nature Communications 2023 Editor's Highlight
- **Articles in Peer-Reviewed Conference Proceedings**
  1. **Towards an Information Theoretic Framework of Context-based Offline Meta-Reinforcement Learning**
     Lanqing Li*, Hai Zhang*, Xinyu Zhang, Shatong Zhu, Yang Yu, Junqiao Zhao, Pheng-Ann Heng
     NeurIPS 2024 Spotlight Paper, top 2.47% (387/15671), top 0.2% (33/15671) in review score
  2. **Class-Conditional Sharpness-Aware Minimization for Deep Long-Tailed Recognition**
     Zhipeng Zhou*, **Lanqing Li***, Peilin Zhao, Pheng-Ann Heng, Wei Gong

CVPR 2023

3. **FOCAL: Efficient Fully-Offline Meta-Reinforcement Learning via Distance Metric Learning and Behavior Regularization**
   Lanqing Li, Rui Yang, Dijun Luo
   ICLR 2021 Seminal paper on offline meta-RL with 120+ citations
4. **Scrutinize What We Ignore: Reining In Task Representation Shift Of Context-Based Offline Meta Reinforcement Learning**
   Hai Zhang, Boyuan Zheng, Tianying Ji, Jinhang Liu, Anqi Guo, Junqiao Zhao, **Lanqing Li**†
   ICLR 2025
5. **On the Pitfall of Mixup for Uncertainty Calibration**
   Deng-Bao Wang, **Lanqing Li**†, Peilin Zhao, Pheng-Ann Heng, Min-Ling Zhang
   CVPR 2023
6. **ImGCL: Revisiting Graph Contrastive Learning on Imbalanced Node Classification**
   Liang Zeng, **Lanqing Li**†, Ziqi Gao, Peilin Zhao, Jian Li
   AAAI 2023
7. **Handling Missing Data via Max-Entropy Regularized Graph Autoencoder**
   Ziqi Gao, Yifan Niu, Jiashun Cheng, Jianheng Tang, Tingyang Xu, Peilin Zhao, **Lanqing Li**†, Fugee Tsung, Jia Li
   AAAI 2023
8. **Local Augmentation for Graph Neural Networks**
   Songtao Liu, Rex Ying, Hanze Dong, **Lanqing Li**†, Tingyang Xu, Yu Rong, Peilin Zhao, Junzhou Huang, Dinghao Wu
   ICML 2022

- **In Submission to Journals and Conferences**

1. **Benchmarking Imbalanced Learning for AI-Aided Drug Discovery**
   Lanqing Li†, Liang Zeng, Ziqi Gao, Shen Yuan, Yatao Bian, Bingzhe Wu, Zhipeng Zhou, Hongteng Xu, Jia Li, Peilin Zhao, Pheng Ann Heng
   Nature Communications (under major revision)
2. **Label-Free Fine-Tuning: Your Protein Language Model is Implicitly a Reward Model**
   Lanqing Li†
   ICLR 2027 (under review)
3. **Be Your Own Teacher: Steering Protein Language Models via Unsupervised Reward Optimization**
   Lanqing Li†, Shentong Mo, Yang Yu, Pheng Ann Heng
   ICLR 2027 (under review) Manuscript featured by BiologyAIDaily and DailyPapers
4. **PepDiT: Structure-Tokenized Diffusion Transformers for Target-Spot Driven Antimicrobial Peptide Generation**
   Shentong Mo, **Lanqing Li**†
   ICLR 2027 (under review)
5. **SaDiT: Efficient Protein Backbone Design via Latent Structural Tokenization and Diffusion Transformers**
   Shentong Mo, **Lanqing Li**†
   ICLR 2027 (under review)

Selected Awards and Honors

Best Poster Presentation, Cell Press Symposia	*2026*
Schmidt Science Fellows - Finalist	*2026*
Outstanding Reviewer, CVPR 2026	*2026*
Global Young Scientists Summit - Finalist	*2025*
Prize for Research Excellence, Zhejiang Lab	*2024*
NSFC Young Scientists Fund (Granted exception as a PhD student)	*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 42nd 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. *Guest lecture on AI for Science*, The Chinese University of Hong Kong, Shenzhen, invited by Prof. Bingyu Cui. (10/2026)
  2. *Aligning Biomolecular Models for Reliable Therapeutic Discovery*, Carnegie Mellon University & MBZUAI, invited by Prof. Eric Xing. (08/2026)
  3. *Aligning Biomolecular Models for Reliable Therapeutic Discovery*, Carnegie Mellon University, invited by Prof. Jian Ma. (07/2026)
  4. *Aligning Biomolecular Models for Reliable Therapeutic Discovery*, Harvard University, invited by Prof. Marinka Zitnik. (06/2026)
  5. *Towards Trustworthy AI For Drug Discovery*, BeOne Medicines, invited by Dr. Lan Hua. (05/2026)
  6. *Trustworthy AI and Applications For Scientific (Biomedical) Discovery*, Shanghai Jiao Tong University, invited by Prof. Peilin Zhao. (12/2025)
  7. *Pre-training paradigm of foundation models for decision making*, Shanghai Jiao Tong University, invited by Prof. Peilin Zhao. (07/2025)
  8. *AI Agent: Principles and Applications*, 1st speaker at CAAI Embodied AI Youth Symposium, invited by Prof. Junqiao Zhao. (12/2023)
  9. *Intelligent Drug Discovery Platform and Its Applications*, presented at the "Computation + Biology" Youth Academic Research Symposium, Zhejiang lab. (09/2023)
  10. *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 CSCI 3100, 3180, 3320, 4130, CUHK *2025-2026*
  2. TA of PHYS 130 Series, UChicago *09/2016-06/2017*
  3. TA of PHYS 14200 Honors Electricity & Magnetism, UChicago *01/2016-03/2016*
  4. TA of PHYS 14100 Honors Mechanics, UChicago *09/2015-12/2015*
  5. 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)

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