

Yanru Qu

Ph.D. in Computer Science - University of Illinois, Urbana-Champaign

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Education

University of Illinois, Urbana-Champaign

Illinois, U.S.

Aug. 2019 - 2021, Aug. 2024 - present

- Ph.D. in Computer Science
- Advisor: Prof. **Ge Liu**, Prof. **Jiaxuan You**, Prof. **Jiawei Han**

Shanghai Jiao Tong University

Shanghai, China

Sep. 2012 - Mar. 2019

- M.S. in Computer Science, GPA: 3.83/4, Major: 3.93/4
- B.E. in Computer Science (IEEE Honored Class), GPA: 86.87/100, Major: 90.59/100
- Advisors: Prof. **Weinan Zhang**, Prof. **Yong Yu**

Research Interests

Generative modeling and representation learning, with a focus on flow/diffusion-based models for AI for Science, including molecular and protein design, as well as foundations in NLP and recommender systems.

Publications (⇒ Google Scholar Profile, cited by 3,800)

Journals.....

Flow Matching Meets Biology and Life Science: A Survey

- Z Li, Z Zeng, X Lin, F Fang, **Yanru Qu**, Z Xu, Z Liu, X Ning, T Wei, G Liu, H Tong, J He
- Accepted to *npj Artificial Intelligence*, 2025

Product-based Neural Networks for User Response Prediction over Multi-field Categorical Data

- **Yanru Qu**, B Fang, W Zhang, R Tang, M Niu, H Guo, Y Yu, X He
- In *ACM Transactions on Information System (TOIS)* (cited by 260+)

Conference (Selected).....

Generative Modeling / AI4Science

Protein Autoregressive Modeling via Multiscale Structure Generation

- **Yanru Qu***, Cheng-Yen Hsieh*, Zaixiang Zheng, Ge Liu, Quanquan Gu
- In Submission to *ICLR'26*

h-MINT: Modeling Pocket-Ligand Binding with Hierarchical Molecular Interaction Network

- **Yanru Qu**, Y Zhang, W Tan, X Kong, X Zhou, C Cheng, M Blanchette, J You, G Liu
- In Submission to *ICLR'26*

Training Free Guided Flow Matching with Optimal Control

- Luran Wang, Chaoran Cheng, Yizhen Liao, **Yanru Qu**, Ge Liu
- In *Proceedings of ICLR'25*

MolCRAFT: Structure-Based Drug Design in Continuous Parameter Space

- **Yanru Qu***, K Qiu*, Y Song*, J Gong, J Han, M Zheng, H Zhou, W Ma
- In *Proceedings of ICML'24* (cited by 50+)

Unified Generative Modeling of 3D Molecules via Bayesian Flow Networks

- Y Song*, J Gong*, **Yanru Qu**, H Zhou, M Zheng, J Liu, W Ma
- In *Proceedings of ICLR'24* (Oral)

NLP / Representation Learning

Coda: Contrast-enhanced and diversity-promoting data augmentation for natural language understanding

- **Yanru Qu**, Dinghan Shen, Yelong Shen, Sandra Sajeew, Jiawei Han, Weizhu Chen
- *In Proceedings of ICLR'21* (cited by 110+)

Dynamically Fused Graph Network for Multi-hop Reasoning

- Yunxuan Xiao*, **Yanru Qu***, Lin Qiu*, Hao Zhou, Lei Li, Weinan Zhang, Yong Yu
- *In Proceedings of ACL'19* (Oral) (cited by 300+)

Recommender System

MAP: A Model-agnostic Pretraining Framework for Click-through Rate Prediction

- J Lin, **Yanru Qu** (corresponding author), W Guo, X Dai, R Tang, Y Yu, W Zhang
- *In Proceedings of KDD'23*

An End-to-End Neighborhood-based Interaction Model for Knowledge-enhanced Recommendation

- **Yanru Qu***, Ting Bai*, Weinan Zhang, Jianyun Nie, Jian Tang
- *In Workshop of DLP-KDD'19* (Best Paper)

Wassertein Distance Guided Representation Learning for Domain Adaptation

- Jian Shen, **Yanru Qu**, Weinan Zhang, Yong Yu
- *In Proceedings of AAAI'18* (cited by 1200+)

Product-based Neural Networks for User Response Prediction

- **Yanru Qu**, Han Cai, Kan Ren, Weinan Zhang, Yong Yu, Ying Wen, Jun Wang
- *In Proceedings of ICDM'16* (Oral) (cited by 870+)

Book & Patent.....

Hands on Natural Language Processing

- Kewei Tu, Xinyu Wang, **Yanru Qu**, Yong Yu
- *Posts & Telecom Press* (2024)

User behavior prediction method and apparatus, and behavior prediction model training method and apparatus

- Ruiming Tang, Minzhe Niu, **Yanru Qu**, Weinan Zhang, Yong Yu
- *US Patent 11,531,867*

Experiences (Selected)

Research Intern at ByteDance Seed

Worked on Protein Design with **Cheng-Yen Hsieh**, **Zaixiang Zheng** and Prof. **Quanquan Gu**

- Submitted a paper to ICLR'26.

San Jose, Ca, US

May. - Dec. 2025

Research Intern at Tsinghua Air

Worked on Molecule Generation with Prof. **Hao Zhou** and Prof. **Weiyang Ma**

- Published a paper in ICLR'24 (oral), and a paper in ICML'24.

Beijing, China

Aug. 2023 - Aug. 2024

Research Intern at D365, Microsoft

Worked on NLP with Dr. **Dinghan Shen**, Dr. **Yelong Shen**, and Dr. **Weizhu Chen**

- Published a paper in ICLR'21 .

Washington, US

May. - Dec. 2020

Research Intern at Mila

Worked on GNN with Prof. **Jian Tang** and Prof. **Jianyun Nie** (UdeM)

- Published a paper and won the **best paper award** of DLP-KDD'19.

Montreal, Canada

June. - Nov. 2018

Student Researcher at APEX Lab, SJTU

Worked with Prof. **Weinan Zhang**, Prof. **Yong Yu**

- Published several papers in ACL, KDD, AAAI, etc.

Shanghai, China

Sep. 2015 - Mar. 2019

Selected Awards

- **2024 Influential New Book Award & 2024 Influential Author Award** (Posts & Telecom Press, China) 2024
- **Best Paper Award** (DLP-KDD'19) 2019
- **Shanghai Outstanding Graduate** (Top 3 in CS Department) 2019
- **National Scholarship for Graduate Students** (Top 3 in CS Department) 2018
- **National Scholarship for Graduate Students** (Top 5 in CS Department) 2017

Open Source Projects

- Implementation of **knowledge-enhanced neighborhood interaction** framework, 60+ stars on github
- Implementation of **product-nets** and **its distributed version**, 500+ stars on github