

# 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 Sajeev, 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)

### Wasserstein 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**

San Jose, Ca, US

May. - Dec. 2025

- Submitted a paper to ICLR'26.

### Research Intern at Tsinghua Air

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

Beijing, China

Aug. 2023 - Aug. 2024

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

### Research Intern at D365, Microsoft

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

Washington, US

May. - Dec. 2020

- Published a paper in ICLR'21 .

### Research Intern at Mila

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

Montreal, Canada

June. - Nov. 2018

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

### Student Researcher at APEX Lab, SJTU

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

Shanghai, China

Sep. 2015 - Mar. 2019

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

## Selected Awards

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- **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

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