

# Yuanqi Du

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## EDUCATIONS

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### George Mason University

*B.S. in Computer Science*

GPA: 4.0/4.0 | Major: 16/18 A+

Fairfax, VA

Aug 2017 - May 2021

### Huaqiao University

*B.S. in Computer Science*

GPA: 4.6/5.0

Xiamen, China

Aug 2016 - Jun 2021

## REPRESENTATIVE PUBLICATIONS

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\* denotes equal contribution, <sup>†</sup> denotes correspondence, full list can be found in [personal website](#) including [in-submissions](#).

### Conference Papers

- **Yuanqi Du**, Xiaojie Guo, Hengning Cao, Yanfang Ye, Liang Zhao. Disentangled Spatiotemporal Graph Generative Model, accepted in *AAAI 2022*, also presented in *NeurIPS 2021 DGMs worksho.*
- **Yuanqi Du\***, Shiyu Wang\*, Xiaojie Guo, et al. GraphGT: Machine Learning Datasets for Graph Generation and Transformation, accepted in *NeurIPS 2021*.
- Xiaojie Guo\*, **Yuanqi Du\***, Liang Zhao. Deep Generative Model for Spatial Networks, published in *KDD 2021*.
- Xiaojie Guo, **Yuanqi Du**, Liang Zhao. Property Controllable Variational Autoencoder via Invertible Mutual Dependence, published in *ICLR 2021*.
- **Yuanqi Du**, Yinkai Wang, Fardina Alam, Yuanjie Lu, Xiaojie Guo, Liang Zhao, and Amarda Shehu. Deep Latent-Variable Models for Controllable Molecule Generation, accepted in *BIBM 2021*.

### Journals

- Xiaojie Guo\*, **Yuanqi Du\***, Sivani Tadepalli, Liang Zhao, Amarda Shehu. Generating Tertiary Protein Structures via an Interpretative Variational Autoencoder, accepted in *Bioinformatics Advances*.

### Workshop Papers

- **Yuanqi Du**, Xian Liu, Shengchao Liu, Jieyu Zhang, Bolei Zhou. Interpreting Molecule Generative Models for Interactive Molecule Discovery, accepted in *ELLIS ML4Molecules workshop 2021 (Oral)*.
- Ziming Liu, Yunyue Chen, **Yuanqi Du**, Max Tegmark. Physics-Augmented Learning: A New Paradigm Beyond Physics-Informed Learning, accepted in *NeurIPS 2021 AI for Science workshop*.

### Workshop Organization

- Payal Chandak, **Yuanqi Du**<sup>†</sup>, Tianfan Fu, Wenhao Gao, Kexin Huang, Shengchao Liu, Ziming Liu, Gabriel Spadon, Max Tegmark, Hanchen Wang, Adrian Weller, Max Welling, Marinka Zitnik (alphabetic order). *AI for Science: Mind the Gaps* workshop, with *NeurIPS 2021*.
- **Yuanqi Du**<sup>†</sup>, Adji Bousso Dieng, Yoon Kim, Rianne Van Den Berg, Yoshua Bengio. *Deep Generative Models for Highly Structured Data*, (tentative) with *ICLR 2022*.

## PROFESSIONAL & RESEARCH EXPERIENCES

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### DP Technology

*Researcher*

Topic: AI for Drug Discovery, Supervisor: Linfeng Zhang

Beijing, China

Oct 2021 - Present

### Princeton University

*Visiting Student*

Princeton, US

Oct 2021 - Present

Topic: Highly Structured Scientific Data Modeling, Advisor: **Adji Bousso Dieng**

**University of Amsterdam**

**Amsterdam, Netherlands**

*Visiting Student (AMLAB & AI4Science)*

*June 2021 - Present*

Topic: Modeling Chemical Systems with Equivariant Neural Nets, Advisor: **Max Welling**

**The Chinese University of Hong Kong**

**Hong Kong**

*Visiting Student (MM Lab)*

*June 2021 - Dec 2021*

Topic: Deep Generative Models for Molecule Generation and Manipulation, Advisor: **Bolei Zhou**

**George Mason University**

**Fairfax, US**

*Research Assistant*

*Jan 2020 - Oct 2021*

Topic: Deep Graph Learning and Molecule/Protein Structure & Dynamic Learning

Advisor: **Liang Zhao, Amarda Shehu**

**Microsoft Research Asia**

**Beijing, China**

*Research Intern (Machine Learning & Computational Biology Group)*

*Nov 2020 - May 2021*

Topic: Protein Structure Prediction, Advisor: **Jianwei Zhu**

**Chinese Academy of Sciences**

**Beijing, China**

*Visiting Student (MIRACLE Group)*

*Aug 2020 - Nov 2020*

Topic: Medical Image Synthesis, Advisors: **S. Kevin Zhou, Hu Han**

## AWARDS & ACHIEVEMENTS

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- MSRA Star of Tomorrow Award 2021
- Distinguished Academic Achievement Award 2021
- Outstanding Graduate Student 2021
- NeurIPS, AIJ AIIDE Travel Award 2020
- NSF REU Fellowship 2019-2020
- Distinguished Undergraduate Research Award 2019-2020
- Distinguished Undergraduate Teaching Assistant Award 2019-2020
- GMU OSCAR Fellowship Summer 2019
- Outstanding Undergraduate Teaching Award 2018-2019
- League of Legends Challenger (world top 0.01%) 2016
- StarCraft II GrandMaster (world top 0.2%) 2015

## TEACHING & MENTORING EXPERIENCES

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**George Mason University**

**Fairfax, US**

*Undergraduate Teaching Assistant*

*Aug 2018 - Dec 2019*

Courses: Object-oriented Programming, Data Structures, Data Mining

**George Mason University**

**Fairfax, US**

*Peer Mentor*

*Feb 2019 - May 2019*

Courses: Research Advisor & Engineering Courses & Careers Services

## PROFESSIONAL SERVICES

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- Reviewer for TPAMI, ICLR, AISTATS, TNNLS, NeurIPS-W, KDD, TKDD, BMVC, CIKM, ICDM, J. Adv. Transp., NeurIPS-AI4Sci, DLG-KDD, IRS-KDD, BioKDD
- Co-organize conferences KDD 2021/AAAI 2021 (Web Team), Co-organize workshops DLG-KDD/AAAI 2021/2022, DeepSpatial-KDD 2020/2021, open-source community (e.g. [GraphGT](#), [GNNBook](#), [Graph4NLP](#), [DeepChem](#))