

# 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 workshop*.
- **Yuanqi Du\***, Shiyu Wang\*, Xiaojie Guo, et al. GraphGT: Machine Learning Datasets for Graph Generation and Transformation, accepted in *NeurIPS 2021 Datasets and Benchmarks track*.
- 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*, with *ICLR 2022*.
- **Yuanqi Du**, Hannes Stärk, Derek Lim, Petar Veličković, Pietro Liò, Michael Bronstein, Stefanie Jegelka, et al. Geometric Deep Learning Conference, in December 2021.

## PROFESSIONAL & RESEARCH EXPERIENCES

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### DP Technology

*Researcher*

Topic: AI for Drug Discovery, Supervisor: **Linfeng Zhang**

Beijing, China

Oct 2021 - Present

<b>Princeton University</b> <i>Visiting Student</i> Topic: Highly Structured Scientific Data Modeling, Advisor: <b>Adji Bousso Dieng</b>	<b>Princeton, US</b> <i>Oct 2021 - Present</i>
<b>University of Amsterdam</b> <i>Visiting Student (AMLAB &amp; AI4Science)</i> Topic: Modeling Chemical Systems with Equivariant Neural Nets, Advisor: <b>Max Welling</b>	<b>Amsterdam, Netherlands</b> <i>June 2021 - Present</i>
<b>The Chinese University of Hong Kong</b> <i>Visiting Student (MM Lab)</i> Topic: Deep Generative Models for Molecule Generation and Manipulation, Advisor: <b>Bolei Zhou</b>	<b>Hong Kong</b> <i>June 2021 - Dec 2021</i>
<b>George Mason University</b> <i>Research Assistant</i> Topic: Deep Graph Learning and Molecule/Protein Structure & Dynamic Learning Advisor: <b>Liang Zhao, Amarda Shehu</b>	<b>Fairfax, US</b> <i>Jan 2020 - Oct 2021</i>
<b>Microsoft Research Asia</b> <i>Research Intern (Machine Learning &amp; Computational Biology Group)</i> Topic: Protein Structure Prediction, Advisor: <b>Jianwei Zhu</b>	<b>Beijing, China</b> <i>Nov 2020 - May 2021</i>
<b>Chinese Academy of Sciences</b> <i>Visiting Student (MIRACLE Group)</i> Topic: Medical Image Synthesis, Advisors: <b>S. Kevin Zhou, Hu Han</b>	<b>Beijing, China</b> <i>Aug 2020 - Nov 2020</i>

## 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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<b>George Mason University</b> <i>Undergraduate Teaching Assistant</i> Courses: Object-oriented Programming, Data Structures, Data Mining	<b>Fairfax, US</b> <i>Aug 2018 - Dec 2019</i>
<b>George Mason University</b> <i>Peer Mentor</i> Courses: Research Advisor & Engineering Courses & Careers Services	<b>Fairfax, US</b> <i>Feb 2019 - May 2019</i>

## 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](#))