

# Yuxuan Song

Tsinghua University – Beijing, China

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## Education

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### Tsinghua University

- Ph.D. in Computer Science and Technology
- Advised by Prof. Wei-Ying Ma.

Beijing, China  
Sep. 2022-present

### Shanghai Jiao Tong University

- Bachelor and Master of Science in Computer Science and Technology
- Research Assistant, Apex Data and Knowledge Management Lab
- Advised by Prof. Yong Yu and Prof. Weinan Zhang.

Shanghai, China  
Sep. 2013-Mar. 2020

## Professional

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Bytedance AI Lab, Researcher(FTE)

May 2020 - Aug. 2021

Microsoft Research Asia, Research Intern

Sep. 2019 - Mar. 2020

## Research Interests

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My research is centered on machine learning, with an emphasis on Deep Generative Models and AI for Science. I'm devoted to developing innovative AI solutions for real-world problems with broad social impacts.

## Publications (\* for Equal Contribution)

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- Y. Qu\*, K. Qiu\*, **Y. Song\***, J. Gong, J. Han, M. Zheng, H. Zhou, W. Ma. MolCRAFT: Structure-Based Drug Design in Continuous Parameter Space. **ICML 2024**.
- **Y. Song\***, J. Gong\*, Y. Qu, M. Zheng, H. Zhou, J. Liu, W. Ma . Unified Generative Modeling of 3D Molecules with Bayesian Flow Networks. **ICLR 2024 (Oral 85/7262)**
- **Y. Song\***, J. Gong\*, M. Xu, Z. Cao, Y. Lan, S. Ermon, H. Zhou, W. Ma . Equivariant Flow Matching with Hybrid Probability Transport for 3D Molecule Generation. **NeurIPS 2023**
- B. Qiang\*, **Y. Song\***, M. Xu, J. Gong, B. Gao, H. Zhou, W. Ma, Y. Lan. Coarse-to-Fine: a Hierarchical Diffusion Model for Molecule Generation in 3D. **ICML 2023**.
- W. Shi\*, **Y. Song\***, H. Zhou, L. Li. Follow Your Path: a Progressive Method for Knowledge Distillation. **ECML/PKDD 2021**.
- **Y. Song**, L. Yu, Z. Cao, Z. Zhou, J. Shen, S. Shao, W. Zhang and Y. Yu. Improving Domain Adaptation with Variational Information Bottleneck. **ECAI 2020**.
- **Y. Song**, N. Miao, H. Zhou, L. Yu and L. Li. Improving Maximum Likelihood Training for Text Generation with Density Ratio Estimation. **AISTATS 2020**.
- **Y. Song**, M. Xu, L. Yu, H. Zhou, S. Shao and Y. Yu. Infomax Neural Joint Source-Channel Coding via Adversarial Bit Flip. **AAAI 2020**.
- **Y. Song**, H. Cai, K. Ren, W. Zhang and Y. Yu. Volume Ranking and Sequential Selection in Programmatic Display Advertising. **CIKM 2017**
- N. Miao, **Y. Song**, H. Zhou and L. Li. Do You Have the Right Scissors? Tailoring Pre-trained Language Models via Monte-Carlo Methods. **ACL 2020**

- Z. Zhou, J. Liang, **Y. Song**, L. Yu, H. Wang, Z. Zhang, W. Zhang and Y. Yu. Lipschitz Generative Adversarial Nets. **ICML 2019**
- G. Lu, Z. Zhou, **Y. Song**, K. Ren and Y. Yu. Guiding the One-to-one Mapping in CycleGAN via Optimal Transport. **AAAI 2019**
- Z. Zhou, H. Cai, S. Rong, **Y. Song**, K. Ren, W. Zhang, Y. Yu and J. Wang. Activation Maximization Generative Adversarial Nets. **ICLR 2018**

## Manuscripts

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- Z. Zhou, **Y. Song**, J. Liang, L. Yu, H. Wang, Z. Zhang, W. Zhang and Y. Yu. Understanding the Effectiveness of Lipschitz Constraint in Training GANs via Gradient Analysis. Technical report. arXiv preprint arXiv:1807.00751, 2018.
- **Y. Song**, M. Xu, Q. Ye, T. Liu. Discriminator Contrastive Divergence: Semi-Amortized Generative Modeling by Exploring Energy of the Discriminator. Technical report. arXiv preprint arXiv:2004.01704, 2020.

## Competitions

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- Our team(AIRFold) win **first place** during 6 months in CAMEO contest of protein folding.

## Honors and Awards

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- **Huawei Scholarship**. 2018
- **CIKM'17/SIGIR Student Travel Grant**. 2017
- **Shanghai Jiao Tong University Outstanding Graduate**. 2017
- **Shanghai Jiao Tong University Excellent Scholarship**. 2014&2015&2016
- **The First Prize in National Mathematical Olympiad in Senior, Liaoning Province**. 2012

## Academic Services

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- **Conference Reviewer**: NeurIPS (2020-2023), ICML(2021-2024), ICLR(2024), AAAI(2020-2022).