

# Zuobai Zhang

Mila – 6666 St Urbain St – Montréal, QC, Canada

☎ +86 18753213029 • ✉ zuobai.zhang@umontreal.ca • 🌐 OXER11.github.io

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## Education

### Mila - Québec AI Institute / Université de Montréal

Montréal, Québec, Canada

Ph.D. in Computer Science

Sept. 2021 – present

- Advisor: Jian Tang
- Research Direction: Graph Representation Learning, Drug Discovery, Protein Science

### Fudan University

Shanghai, China

B.S. in Computer Science (Honor Class)

Sept. 2017 – Jun. 2021

- Advisor: Zhongzhi Zhang
- Research Direction: Graph Mining, Network Science, Spectral Graph Theory
- (First three years) GPA: 3.93/4.0, Major GPA: 3.99/4.0, Ranking: 1/145
- (Overall) GPA: 3.86/4.0, Ranking: 1/145

## Internship

### ByteDance Inc.

Shanghai, China

Machine Learning Engineering Intern

Sept. 2020 – Jan. 2021

- Worked in Data-Rec Shanghai Group led by Yitan Li.
- Designed machine learning algorithms to improve the recommender system of Toutiao and developed new features in real-world products.

## Preprints

- **DiffPack: A Torsional Diffusion Model for Autoregressive Protein Side-Chain Packing.**  
Yangtian Zhang\*, **Zuobai Zhang\***, Bozitao Zhong, Sanchit Misra, Jian Tang
- **Pre-Training Protein Encoder via Siamese Sequence-Structure Diffusion Trajectory Prediction.**  
**Zuobai Zhang\***, Minghao Xu\*, Aurélie Lozano, Vijil Chenthamarakshan, Payel Das, Jian Tang
- **TorchDrug: A Powerful and Flexible Machine Learning Platform for Drug Discovery.**  
Zhaocheng Zhu, Chence Shi, **Zuobai Zhang**, Shengchao Liu, Minghao Xu, Xinyu Yuan, Yangtian Zhang, Junkun Chen, Huiyu Cai, Jiarui Lu, Chang Ma, Runcheng Liu, Louis-Pascal Xhonneux, Meng Qu, Jian Tang
- **A Roadmap for Big Model.**  
*I'm a co-first author of this paper.*

## Publications

- **FusionRetro: Molecule Representation Fusion via In-context Reactions for Retrosynthetic Planning**  
Songtao Liu, Zhengkai Tu\*, Minkai Xu\*, **Zuobai Zhang\***, Peilin Zhao, Jian Tang, Rex Ying, Lu Lin, Dinghao Wu  
ICML 2023
- **Enhancing Protein Language Models with Structure-based Encoder and Pre-Training.**  
**Zuobai Zhang**, Minghao Xu, Vijil Chenthamarakshan, Aurélie Lozano, Payel Das, Jian Tang  
ICLR 2023 Machine Learning for Drug Discovery Workshop
- **Protein Representation Learning by Geometric Structure Pretraining.**  
**Zuobai Zhang**, Minghao Xu, Arian Jamasb, Vijil Chenthamarakshan, Aurelie Lozano, Payel Das, Jian Tang  
ICLR 2023  
ICML 2022 Pre-Training Workshop

- **PEER: A Comprehensive and Multi-Task Benchmark for Protein Sequence Understanding.**  
Minghao Xu\*, **Zuobai Zhang\***, Jiarui Lu, Zhaocheng Zhu, Yangtian Zhang, Chang Ma, Runcheng Liu, Jian Tang  
*NeurIPS 2022 Datasets and Benchmarks Track*
- **Effects of Stubbornness on Opinion Dynamics.**  
Wanyue Xu, Liwang Zhu, Jiale Guan, **Zuobai Zhang**, Zhongzhi Zhang  
*CIKM 2022*
- **Neural-Symbolic Models for Logical Queries on Knowledge Graphs.**  
Zhaocheng Zhu, Mikhail Galkin, **Zuobai Zhang**, Jian Tang  
*ICML 2022*
- **Structured Multi-task Learning for Molecular Property Prediction.**  
Shengchao Liu, Meng Qu, **Zuobai Zhang**, Huiyu Cai, Jian Tang  
*AISTATS 2022, NeurIPS AI for Science Workshop 2021*
- **Bi-harmonic Distance-Based Performance Metric for Second-Order Noisy Consensus Networks.**  
Yuhao Yi, Bingjia Yang, **Zuobai Zhang**, Wanyue Xu, Zhongzhi Zhang, Stacy Patterson  
*IEEE Transactions on Information Theory*
- **Neural Bellman-Ford Networks: A General Graph Neural Network Framework for Link Prediction.**  
Zhaocheng Zhu, **Zuobai Zhang**, Louis-Pascal Xhonneux, Jian Tang  
*NeurIPS 2021*
- **Learning Interpretable Cellular and Gene Signature Embeddings from Single-Cell Transcriptomic Data.**  
Yifan Zhao\*, Huiyu Cai\*, **Zuobai Zhang**, Jian Tang, Yue Li  
*Nature Communications*
- **Minimizing Spectral Radius of Non-Backtracking Matrix by Edge Removal.**  
**Zuobai Zhang**, Zhongzhi Zhang, Guanrong Chen  
*CIKM 2021*
- **Coherence Scaling of Noisy Second-Order Scale-Free Consensus Networks.**  
Wanyue Xu, Bin Wu, **Zuobai Zhang**, Zhongzhi Zhang, Haibin Kan, Guanrong Chen  
*IEEE Transactions on Cybernetics*
- **Opinion Dynamics Incorporating Higher-Order Interactions.**  
**Zuobai Zhang**, Wanyue Xu, Zhongzhi Zhang, Guanrong Chen  
*ICDM 2020 (short paper)*
- **Power-Law Graphs Have Minimal Scaling of Kemeny Constant for Random Walks.**  
Wanyue Xu, Yibin Sheng, **Zuobai Zhang**, Haibin Kan, Zhongzhi Zhang  
*The Web Conference 2020*
- **Fast Approximation of Coherence for Second-Order Noisy Consensus Networks.**  
**Zuobai Zhang**, Wanyue Xu, Yuhao Yi, Zhongzhi Zhang  
*IEEE Transactions on Cybernetics*
- **Nearly Linear Time Algorithm for Mean Hitting Times of Random Walks on a Graph.**  
**Zuobai Zhang**, Wanyue Xu, Zhongzhi Zhang  
*WSDM 2020*

## Selected Projects

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- **TorchProtein: A Flexible Machine Learning Library for Protein Science.** (with TorchProtein team)  
A machine learning library for protein science based on TorchDrug, providing representation learning models for both sequences and structures, and fundamental protein tasks like function prediction, structure prediction.  
[Homepage] [Github] [Twitter]
- **TorchDrug: A Powerful Machine Learning Platform for Drug Discovery.** (with TorchDrug team)

A machine learning platform designed for drug discovery, covering techniques from graph machine learning, deep generative models to reinforcement learning.

[\[Homepage\]](#)   [\[Github\]](#)   [\[Twitter\]](#)

## Honors & Awards

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Outstanding Undergraduates Graduates of Shanghai	Jun. 2021
Scholarships for Outstanding Academic Individuals at Fudan University	Dec. 2020
Shanghai Scholarship (Top 1%)	Oct. 2020
SenseTime Scholarship (29 undergrads from China)	Jan. 2020
Chinese National Scholarship (Top 1%)	Oct. 2019
Chun Tsung Scholar Program	Apr. 2019
Wish Scholarship	May 2019
Chinese National Scholarship (Top 1%)	Oct. 2018
Gold Medal, ACM-ICPC Asia Regional Contest EC-Final	Dec. 2017
Gold Medal, ACM-ICPC Asia Regional Contest Qingdao Site	Nov. 2017
Silver Medal, National Olympiad in Informatics, National Finals	Jul. 2016
Gold Medal, Winter Camp of National Olympiad in Informatics	Jan. 2016
First Prize (2nd place), National Olympiad in Informatics, Shandong Division	Nov. 2015

## Skills

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- **Programming Languages:** Python, C/C++,  $\text{\LaTeX}$ , Julia, JavaScript, MATLAB, HTML
- **Language:** Chinese-Native, English-Fluent (GRE: 162+169+4.0)