

HUIYU CAI

Mila & University of Montreal

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EDUCATION

- Quebec AI Institute (Mila) & University of Montreal (UdeM)** *Sep. 2021 - Present*
Department of Computer Science and Operations Research (DIRO) Overall GPA: 4.30/4.30
Third year PhD candidate supervised by Prof. Jian Tang, working on applications of generative models and geometric deep learning to biomolecular interaction modeling.
- Peking University (PKU)** *Sep. 2017 - Jul. 2021*
School of Electronic Engineering and Computer Science (EECS) Overall GPA: 3.60/4.00
Awarded **Excellent Graduate in Beijing**.
- Peking University (PKU)** *Sep. 2016 - Jun. 2017*
College of Chemistry and Molecular Engineering (CCME) Overall GPA: 3.68/4.00
Ranking: **Top 5%** in CCME, 2016-2017. Note: I changed my major to EECS after Jun 2017.

TECHNICAL STRENGTHS

- Computer Languages** C/C++ (gdb), Python (pdb), Java, Bash, R*, Assembly Language*, JavaScript (Vue)*, Matlab*, SQL*
- Computing Frameworks** Spark*, MapReduce*, OpenMP*, MPI*
- Python Libraries** NumPy, Sci-kit Learn, Pandas, Matplotlib, Seaborn, PyTorch, Flask, SQLAlchemy, ScanPy, RDKit, PyMOL, BioPython, AbNumber, Re*, TensorFlow*, Sympy*, BeautifulSoup*, Selenium*, PyRosetta*
- English Fluency** TOEFL iBT 114 (Reading 30, Listening 30, Speaking 27, Writing 27)
GRE Verbal 157, Quantitative 170, Analytical Writing 3.5
IELTS 8.0 (Listening 8.5, Reading 8.0, Writing 7.0, Speaking 7.5)
- Mathematics** Mathematical Analysis, Set and Graph Theory, Probability Theory and Statistics, Linear Algebra, Stochastic Processes, Convex Analysis and Optimization Methods, Machine Learning Theory
- * I learned the basics and have used them in projects but am no expert

PUBLICATIONS

- Huiyu Cai***, Zuobai Zhang*, Mingkai Wang*, Bozita Zhong*, Yanling Wu, Tianlei Ying, Jian Tang. Pretrainable Geometric Graph Neural Network for Antibody Affinity Maturation, *In submission*. *Equal contribution
- Yangtian Zhang*, **Huiyu Cai***, Chence Shi, Jian Tang. E3Bind: An End-to-End Equivariant Network for Protein-Ligand Docking, *ICLR*, **2023**. *Equal contribution
- Shengchao Liu, Meng Qu, Zuobai Zhang, **Huiyu Cai**, Jian Tang. Structured Multi-task Learning for Molecular Property Prediction, *AISTATS*, **2022**.
- Meng Qu*, **Huiyu Cai***, Jian Tang. Neural Structured Prediction for Inductive Node Classification. *ICLR*, **2022** (oral). *Equal contribution
- Yifan Zhao*, **Huiyu Cai***, Zuobai Zhang, Jian Tang, Yue Li. Learning interpretable cellular and gene signature embeddings from single-cell transcriptomic data, *Nature Communications*, **2021**. *Equal contribution
- Yitao Cai, **Huiyu Cai**, Xiaojun Wan. Multi-Modal Sarcasm Detection in Twitter with Hierarchical Fusion Model, *ACL*, **2019**.

Jingjia Liu, Yuting Zhang, **Huiyu Cai**, Juan Yang. TEMPO and Its Derivatives in Organic Redox-Flow Batteries, *University Chemistry*, **2017**, 32(11): 32-44.

RESEARCH INTERESTS

Deep Generative Models, Geometric Deep Learning, Representation Learning, AI for Drug Discovery

AWARDS AND HONORS

Excellent Graduate in Beijing, 2021

Excellent Graduate of Peking University, 2021

Leo Koguan Scholarship (1 out of 150), 2017

Leo Koguan Scholarship (1 out of 62), 2020

Founder Scholarship (2 out of 61), 2019

Second Prize, ACM-ICPC PKU campus competition, 2018

First Prize, 29th Chinese Chemistry Olympiad (Preliminary), 2015

First Prize, 28th Chinese Chemistry Olympiad (Preliminary), 2014

HOBBIES

A cappella singing and arrangement (I was the music director of Paca Vocal Group at Peking University and was involved in the production of two albums)

Watching Sci-Fi (especially the Star Trek series)

Hiking / Stargazing / Swimming / Travelling / Ping pong