

Meng Liu

Ph.D. Student
Department of Computer Science & Engineering
Texas A&M University

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Research Interests

Graph Deep Learning: graph neural networks, expressiveness, large-scale graphs, 3D graphs, open-source library.

AI for Science: molecular property prediction, molecule generation, protein-ligand binding.

Generative Modeling: energy-based models, flow models.

Education

Texas A&M University, College Station, TX, USA
Ph.D., Department of Computer Science & Engineering
Advisor: [Prof. Shuiwang Ji](#)

Sep 2019 – Present

Tsinghua University, Beijing, CHINA
B.E., Department of Electronic Engineering
Advisor: [Prof. Liangrui Peng](#)
Thesis: A Deep Learning Method for Multi-lingual Scene Text Detection

Aug 2015 – Jul 2019

Professional Experiences

Meta AI, Menlo Park, CA, USA
Research Intern
Worked on graph-based recommendation over billion-scale graphs.
Mentor: [Xing Wang](#)

May 2022 – Aug 2022

Fujitsu Research of America, Sunnyvale, CA, USA
Research Intern
Worked on applying transformers on graphs.
Mentor: [Kanji Uchino](#)

Jun 2021 – Aug 2021

Owlii (acquired by Kwai Inc.), Beijing, CHINA
R&D Intern
Mentor: [Yi Xu](#)

May 2018 – Aug 2018

Publications [[Google Scholar](#)]

* indicates equal contribution.

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| [ICML 2022] | Generating 3D Molecules for Target Protein Binding
Meng Liu , Youzhi Luo, Kanji Uchino, Koji Maruhashi, and Shuiwang Ji
<i>International Conference on Machine Learning (ICML)</i> , 2022
Oral/Long Presentation (118/5630=2.1% acceptance rate) |
| [ICML 2022] | GraphFM: Improving Large-Scale GNN Training via Feature Momentum
Haiyang Yu*, Limei Wang*, Bokun Wang*, Meng Liu , Tianbao Yang, and Shuiwang Ji
<i>International Conference on Machine Learning (ICML)</i> , 2022 |
| [Bioinformatics] | Advanced graph and sequence neural networks for molecular property prediction and drug discovery
Zhengyang Wang*, Meng Liu* , Youzhi Luo*, Zhao Xu*, Yaochen Xie*, Limei Wang*, Lei Cai*, Qi Qi, Zhuoning Yuan, Tianbao Yang, and Shuiwang Ji
<i>Bioinformatics</i> , 2022
Rank #1 on AI Cures open challenge for COVID-19 |
| [ICLR 2022] | Spherical Message Passing for 3D Molecular Graphs
Yi Liu*, Limei Wang*, Meng Liu , Yuchao Lin, Xuan Zhang, Bora Oztekin, and Shuiwang Ji |

- [SDM 2022]** **Neighbor2Seq: Deep Learning on Massive Graphs by Transforming Neighbors to Sequences**
Meng Liu and Shuiwang Ji
SIAM International Conference on Data Mining (SDM), 2022
- [TPAMI]** **Non-Local Graph Neural Networks**
Meng Liu*, Zhengyang Wang*, and Shuiwang Ji
IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI), 2021
- [NeurIPS-W 2021]** **Fast Quantum Property Prediction via Deeper 2D and 3D Graph Networks**
Meng Liu*, Cong Fu*, Xuan Zhang, Limei Wang, Yaochen Xie, Hao Yuan, Youzhi Luo, Zhao Xu, Shenglong Xu, and Shuiwang Ji
AI4Science Workshop at NeurIPS, 2021
Awardee of KDD Cup 2021 on OGB-LSC
- [JMLR]** **DIG: A Turnkey Library for Diving into Graph Deep Learning Research**
Meng Liu*, Youzhi Luo*, Limei Wang*, Yaochen Xie*, Hao Yuan*, Shurui Gui*, Haiyang Yu*, Zhao Xu, Jingtun Zhang, Yi Liu, Keqiang Yan, Haoran Liu, Cong Fu, Bora Oztekin, Xuan Zhang, and Shuiwang Ji
Journal of Machine Learning Research (JMLR), 2021
- [ICLR-W 2021]** **GraphEBM: Molecular Graph Generation with Energy-Based Models**
Meng Liu, Keqiang Yan, Bora Oztekin, and Shuiwang Ji
EBM Workshop at ICLR, 2021
- [KDD 2020]** **Towards Deeper Graph Neural Networks**
Meng Liu, Hongyang Gao, and Shuiwang Ji
ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD), 2020

Professional Services

Session Chair

International Conference on Machine Learning (**ICML**) 2022

Program Committee Member | Reviewer

Annual Conference on Neural Information Processing Systems (**NeurIPS**) 2021, 2022
 NeurIPS Track Datasets and Benchmarks 2022
 International Conference on Machine Learning (**ICML**) 2021, 2022
 ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD**) 2021, 2022
 International Conference on Learning Representations (**ICLR**) 2020, 2021, 2022
 IEEE Conference on Computer Vision and Pattern Recognition (**CVPR**) 2022
 European Conference on Computer Vision (**ECCV**) 2022
 SIAM International Conference on Data Mining (**SDM**) 2022
 Deep Generative Models for Highly Structured Data Workshop @ ICLR2022 2022
 Machine Learning on Graphs Workshop @ WSDM2022 2022
 AI4Science Workshop @ NeurIPS2021 @ ICML2022 2021, 2022
 IEEE Transactions on Pattern Analysis and Machine Intelligence (**TPAMI**)
 Transactions on Machine Learning Research (**TMLR**)
 Neurocomputing
 IEEE Transactions on Neural Networks and Learning Systems (**TNNLS**)
 BMC Bioinformatics

Talks & Guest Lectures

Generating 3D Molecules for Target Protein Binding ICML, 2022
 Generating 3D Molecules for Target Protein Binding Fujitsu, 2022
 Deep Learning on Graphs BMI 6334, UTHealth, 2021
 Deep Learning on Graphs CSCE 636, Texas A&M University, 2021

Graph Neural Networks
Graph Neural Networks
Towards Deeper Graph Neural Networks

BMI 6334, UTHealth, 2020
CSCE 636, Texas A&M University, 2020
KDD, 2020

Scholarships, Awards, & Honors

ICML Outstanding Reviewer	2022
ICML Travel Award	2022
Travel Award for AI4Science Workshop @ NeurIPS	2021
Runner-up award of KDD Cup on Open Graph Benchmark Large-Scale Challenge (OGB-LSC)	2021
KDD Student Travel Award	2020
Comprehensive Excellence Scholarship, Tsinghua University	2017