

# Meng Liu

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

E-mail: [mengliu@tamu.edu](mailto:mengliu@tamu.edu)  
Homepage: [mengliu1998.github.io](https://mengliu1998.github.io)

---

## Research Interests

**Graph Deep Learning:** graph neural networks, expressiveness, large-scale graphs, 3D graphs, open-source library.  
**AI for Drug Discovery:** molecular property prediction, molecule generation, protein-ligand binding.  
**Generative Modeling:** energy-based models, flow models.

## Education

**Texas A&M University**, College Station, TX, USA Sep 2019 – Present  
Ph.D., Department of Computer Science & Engineering  
Advisor: [Prof. Shuiwang Ji](#)

**Tsinghua University**, Beijing, CHINA Aug 2015 – Jul 2019  
B.E., Department of Electronic Engineering  
Advisor: [Prof. Liangrui Peng](#)  
Thesis: A Deep Learning Method for Multi-lingual Scene Text Detection

## Professional Experiences

**Meta**, Menlo Park, CA, USA May 2022 – Aug 2022  
Research Intern  
AI Platform.  
Mentor: [Xing Wang](#)

**Fujitsu Research of America**, Sunnyvale, CA, USA Jun 2021 – Aug 2021  
Research Intern  
Worked on applying transformers on graphs.  
Mentor: [Kanji Uchino](#)

**Owlii** (acquired by Kwai Inc.), Beijing, CHINA May 2018 – Aug 2018  
R&D Intern  
Mentor: Yi Xu

## Publications [[Google Scholar](#)]

\* indicates equal contribution.

- [ICML 2022] **Generating 3D Molecules for Target Protein Binding**  
Meng Liu, Youzhi Luo, Kanji Uchino, Koji Maruhashi, and Shuiwang Ji  
*International Conference on Machine Learning (ICML), 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  
*International Conference on Machine Learning (ICML), 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  
*Bioinformatics, 2022*
- [ICLR 2022] **Spherical Message Passing for 3D Molecular Graphs**  
Yi Liu\*, Limei Wang\*, Meng Liu, Yuchao Lin, Xuan Zhang, Bora Oztekin, and Shuiwang Ji  
*International Conference on Learning Representations (ICLR), 2022*

- [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  
*Runner-up award of KDD Cup on OGB-LSC*  
*AI4Science Workshop at NeurIPS, 2021*
- [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

### **Program Committee Member | Reviewer**

Annual Conference on Neural Information Processing Systems ( <b>NeurIPS</b> )	2021, 2022
International Conference on Machine Learning ( <b>ICML</b> )	2021, 2022
ACM SIGKDD Conference on Knowledge Discovery and Data Mining ( <b>KDD</b> )	2021, 2022
International Conference on Learning Representations ( <b>ICLR</b> )	2020, 2021, 2022
IEEE Conference on Computer Vision and Pattern Recognition ( <b>CVPR</b> )	2022
European Conference on Computer Vision ( <b>ECCV</b> )	2022
SIAM International Conference on Data Mining ( <b>SDM</b> )	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 ( <b>TPAMI</b> )	
Transactions on Machine Learning Research ( <b>TMLR</b> )	
Neurocomputing	
IEEE Transactions on Neural Networks and Learning Systems ( <b>TNNLS</b> )	
BMC Bioinformatics	

## Talks & Guest Lectures

Deep Learning on Graphs	BMI 6334, UTHealth, 2021
Deep Learning on Graphs	CSCE 636, Texas A&M University, 2021
Graph Neural Networks	BMI 6334, UTHealth, 2020
Graph Neural Networks	CSCE 636, Texas A&M University, 2020
Towards Deeper Graph Neural Networks	KDD 2020

## Scholarships, Awards, & Honors

Travel Award for AI4Science Workshop @ NeurIPS	2021
Runner-up award of KDD Cup on Open Graph Benchmark Large-Scale Challenge (OGB-LSC)	2021

