# Guikun Xu

AI for Science · Molecular Machine Learning · Deep Generative Models

*School of Computing and Artificial Intelligence, Xipu Campus, Southwest Jiaotong University*

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## Education

**Southwest Jiaotong University (SWJTU)** — *Chengdu, China*

**M.S.** in Computer Science and Technology (Expected) — *Sep. 2022 - Present*

- **Mentors:** Professor Yan Yang and Assistant Researcher Yongquan Jiang
- **GPA**: 3.73/4
- **Main Courses:** Matrix Analysis (96.5/100); Mathematical Statistics and Multivariate Statistics (86/100); Optimization Theory and Methods (92/100); Computer Vision (85.6/100)

**Southwest Petroleum University (SWPU)** — *Chengdu, China*

**B.S.** in Electronic Information Science and Technology — *Sep. 2018 - Jul. 2022*

- **GPA**: 3.48/5.0

## Experience

**Deep Learning-Based Research on Molecular Conformation** — *Chengdu, China*

Southwest Jiaotong University (SWJTU) — *Sep. 2022 - Present*

- Our paper has been accept as a Spotlight Presentation [Top 5%] in The Twelfth International Conference on Learning Representations(ICLR 2024)

**Undergraduate Dissertation: Research on Image Classification Models Based on Deep Learning** — *Chengdu, China*

Southwest Petroleum University (SWPU) — *Jan. 2022 - Jun. 2022*

- Enhanced proficiency in using the PyTorch deep learning framework and gained comprehensive understanding of training strategies for supervised learning.

**Production Internship: Smart Home Simulation System** — *Chengdu, China*

Southwest Petroleum University (SWPU) — *Jun. 2021 - Jul. 2021*

- Responsible for code development in the project: Building the server (development board + C) and client (QT).

**College Students' Innovation and Entrepreneurship Training Program** — *Chengdu, China*

Southwest Petroleum University (SWPU) — *2019 - 2020*

- In our project "Research on Deep Learning-Based Automatic Navigation Semantic Segmentation System", I have gained an understanding of the basic overview of deep learning and acquired preliminary knowledge about the PyTorch deep learning framework.

## Publications

**GTMGC: Using Graph Transformer to Predict Molecule's Ground-State Conformation** — *ICLR2024 (spotlight)*

Guikun Xu, Yongquan Jiang, Pengchuan Lei, Yan Yang, Jim Chen — *2024*

- **Keywords**: molecular conformation prediction, molecule modeling, graph neural network, graph transformer
- **TL;DR:** We propose a Graph-Transformer network which uses a novel self-attention mechanism we developed for molecular structure modeling, achieving SOTA performance in predicting a molecule's ground-state 3D conformation from its 2D topology graph.

## Skills

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|---|---|
| **DL Frameworks** | PyTorch, TensorFlow, PaddlePaddle |
| **Programming Languages** | Python, C/C++, JAVA, LaTeX |
| | Chinese, English (CET-6 552/710) |

## Honors & Awards

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| 2023.10 | **2nd Class Academic Scholarship**, Southwest Jiaotong University (SWJTU). | *Chengdu, China* |
| 2022.10 | **2nd Class Academic Scholarship**, Southwest Jiaotong University (SWJTU). | *Chengdu, China* |
| 2021.10 | **Certificate of Completion and Second Prize for Provincial-level College Students' Innovation and Entrepreneurship Training Program in 2020**, Southwest Petroleum University (SWPU). | *Chengdu, China* |