# 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*

- Currently, I am dedicated to researching accelerated algorithms for the generation of molecular conformational ensembles. In recent years, diffusion-based algorithms for generating molecular conformational ensembles have become the mainstream approach in this field. However, the original diffusion model requires multiple steps of denoising, which significantly slows down the generation process. Therefore, the challenge lies in finding a way to accelerate the speed of the molecular conformational ensemble generation algorithm while ensuring high quality results. To address this issue, I am exploring and developing new algorithms and techniques with the aim of significantly improving the algorithm's execution speed, while maintaining high generation quality.
- Successfully, a network based on the Graph Transformer architecture has been constructed, achieving end-to-end prediction from the 2D topology of molecules to their 3D ground-state conformations, and attaining the state-of-the-art performance. In algorithm design, a novel and effective self-attention module has been proposed for 3D molecular structure modeling. This module greatly retains the practicality and elegance of the self-attention mechanism in the original Transformer network, while also exhibiting remarkable performance, making it easy to implement and quickly transfer to other molecular modeling tasks. This research achievement has been accepted by the 12th International Conference on Learning Representations (ICLR 2024) and selected as a Spotlight Presentation [Top 5%].

### Undergraduate Dissertation: Research on Image Classification Models Based on Deep Learning

*Chengdu, China*

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

- I have mastered the basic usage of PyTorch deep learning framework and the training and tuning process for image classification tasks in computer vision. As a result, I have gained in-depth understanding and practical experience in implementing classic vision models such as LeNet, AlexNet, VGG, and ResNet.

## 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

**DL Frameworks** PyTorch, TensorFlow, PaddlePaddle

**Programming** Python, C/C++, JAVA, LaTeX

**Languages** Chinese, English (CET-6 552/710)

## Honors & Awards

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*