

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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“Believe, but don’t expect.”

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

Skills

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

Experience

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.

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

Publications

GTMG: 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.