Jiawei Zhan

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EDUCATION

- **University of Chicago** | Chicago, IL — Expected Dec. 2025
  Ph.D. in Quantum Science and Engineering — GPA: 3.93/4.0
- **Georgia Institute of Technology** | Atlanta, GA — Expected Jul. 2024
  M.S. in Computer Science — GPA: 4.0/4.0
- **University of Science and Technology of China** | Hefei, China — Sep. 2016 - Jul. 2020
  B.S. in Applied Physics — GPA: 3.72/4.0

SELECTED PUBLICATION

- **J. Zhan,** M. Govoni, G. Galli, *Nonempirical Range-Separated Hybrid Functional with Spatially Dependent Screened Exchange*, J. Chem. Theory Comput. (2023) (A top-tier journal in computational and theoretical chemistry)
- S. Yang, I. Bier, W. Wen, **J. Zhan**, S. Moayedpour, and N. Marom, *Ogre: A Python Package for Molecular Crystal Surface Generation with Applications to Surface Energy and Crystal Habit Prediction*, J Chem Phys. (2020)

INDUSTRIAL EXPERIENCE

ByteDance (TikTok) | Machine Learning Research Scientist Intern — Jun. 2023 – Sep. 2023

Project**: Predicting Physical Models with Uncertainty-Aware Graph Neural Networks**

- Designed a graph representation for many-body systems, reducing computational time and storage needs.
- Implemented a Graph Neural Network with Janossy Pooling for improved pattern extraction from graph data.
- Developed a multithread dataset with data distribution scheme to streamline data loading, enabling training on datasets up to ~TB with balanced GPU load. This reduced training cost from minutes to seconds per epoch.
- Estimating the posterior Gaussian distribution of neural network's weights by approximating the low-rank covariance matrix, enabling efficient out-of-domain data detection and prediction risk calibration.

ACAMEMIC EXPERIENCE

The University of Chicago | Research Assistant — Apr. 2023 – Present

Project**: High-Dimensional Embedding and Transformer-Based Model for Quantum System Analysis**

- Developed CUDA kernels for k-subgraph clustering, realizing a 1000x speedup compared to serial methods.
- Devised a physical-constraint structural embedding for local radial information representation.
- Utilized Transformers to capture complex quantum system dependencies, achieving superior performance with less training data than state-of-the-art models and maintaining robustness to major structural perturbations.
- Designed active learning workflow based on numerical evaluation of uncertainties using ensemble learning.

The University of Chicago | Research Assistant — Feb. 2021 – May. 2023

Project**: Optimizing Large-Scale Parallel Algorithms for Complex Systems Modeling**

- Employed and assessed mathematical models to capture essential physical interactions within complex systems.
- Used Fast Fourier Transform and Monte Carlo with OpenMP and MPI for scalable integral evaluations.
- Computed eigenvalue spectra of high-dimensional matrices using iterative projection.

Carnegie Mellon University | Research Assistant — Jul. 2019 – Sep. 2019

Project**: Designing Symmetry-Preserving Neural Network for Multi-Objective Structural Optimization**

- Designed a specialized graph algorithm for efficient conversion between external and internal coordinates.
- Derived a symmetry preserving GNN model for predicting the optimal structure of fragmented system.
- Applied Gaussian Processes to determine the Pareto optimum in multi-objective structural relaxation.

ADDITIONAL INFORMATION

Honors & Awards: 2018, 2019 Outstanding Student Scholarship（USTC)

Leadership & Activity: Lead Method Development Sub-group at Galli's group (UChicago)

Computer Skills: Python, C/C++, MATLAB, Mathematica; CUDA, OpenMP, MPI; Bash; LaTeX, Markdown