KANGQI YANG

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EDUCATION

School of Materials Science and Engineering, Georgia Institute of Technology **Atlanta, GA, USA**
M.S. in Computational Science and Engineering *Aug. 2025 – May 2027 (Expected)*

- **GPA:** 4.0 / 4.0
- **Coursework:** Computational Data Analysis (Machine Learning, PyTorch), Computational Modeling & Simulation, Knowledge-Based AI (reasoning, planning, agents); Computational Statistics (in progress), Large Language Models (in progress), Comp Sci & Engr Algorithms (in progress).

School of Chemistry, Sun Yat-sen University **Guangzhou, China**
B.Eng. in Macromolecular Material and Engineering *Sep. 2021 – June 2025*

- **GPA:** 3.7 / 4.0, **rank:** 1 / 37
- **Research Focus:** Theoretical and Computational Chemistry; Materials Calculations and Simulations
- **Honors:** 2023 & 2024 National Scholarship (Top 0.2%); 2022-2024 First Prize in Outstanding Students Scholarship (Top 5%); 2022 First Prize in National Mathematics Competition (Top 5%)

RESEARCH & PROJECT EXPERIENCE

Explore the Computational Method for Excited-State Proton Transfer (PT) in the Liquid Phase
NYU Shanghai - Summer Research Intern, Supervised by Dr. Xiang Sun *July 2024 - Sep. 2024*

- Built machine learning-augmented molecular dynamics pipelines to learn representations of molecular configurations and energy surfaces from first-principles simulations (5K+ structures).
- Integrated deep neural potential models (DeePMD) with LAMMPS to enable data-efficient prediction of physicochemical properties and reaction mechanisms in excited-state proton transfer.
- Designed Python-based data preprocessing, validation, and visualization pipelines for large-scale scientific datasets, improving simulation throughput by 50% while reducing computational cost by 60%.

Thermal Conduction Transport in Organic-Inorganic Hybrid Materials
Sun Yat-sen University - Research Project Lead, Supervised by Dr. Wen Shi *Sep. 2023 - May 2025*
Selected by National Undergraduate Training Program for Innovation and Entrepreneurship (top 1% of college)

- Established the mapping relationship between energy level and molecular structures, constructed a fine-tuned deep potential energy ML model to quantitatively predict the potential surface in metal-organic frameworks; achieving high accuracy and efficiency, while significantly reducing costs against conventional methods
- Applied Fourier's law and Non-Equilibrium Molecular Dynamics (NEMD) to compute thermal conductivity of organic-inorganic hybrid materials iteratively in complex systems
- Leveraged Python scripts to automate the thermal conductivity prediction workflow; streamlined procedures for structural input, dataset construction, training, and computation; increased efficiency by 40%

Quantitative Structure-Activity Relationship (QSAR) Study of Cancer Immunotherapy
Sun Yat-sen University – Course Project, Supervised by Dr. Yong Shen *Dec. 2023 - Jan. 2024*

- Developed a QSAR model and employed stepwise linear regression to investigate the relationship between molecular structures and inhibitory activity using SPSS, with R^2 values of 0.678
- Conducted feature engineering and correlational analysis in Python, and identified 3 key indicators driving compound activity at a significant confidence level, resulting in a 50% increase in efficiency
- Applied the model to predict and design new compounds for drugs with 30% improved inhibitory potential

PUBLICATIONS

Kangqi Yang, Xiaomei Wu, Wen Shi. "A First-Principles-Trained Deep Learning Framework for Predicting Thermal Conductivity in Two-Dimensional Metal-Organic Frameworks." Manuscript in preparation

PROFESSIONAL SKILLS

Programming Languages: Python (NumPy, PyTorch), C++, MATLAB
Technical Skills & Tools: Bash Shell, LaTeX, HTML, CSS, SQL