

Guanyao Mao

(Personal Website: <https://wdsdz.github.io/>)

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EDUCATION

Fudan University	ShangHai, China	
<i>Bachelor of Science in Optoelectronic Information and Engineering</i>		08/2022- Present
Stanford University	Palo Alto, CA, USA	
<i>IHP Honors Program (Culminative GPA: 4.0)</i>		06/2025- 08/2025
<ul style="list-style-type: none">• Cumulative GPA: 88/100• Honors: Huatai Securities Science and Technology Scholarship (First Prize) Puyuan Talent Scholarship (Second Prize) Haoersai Science & Technology Scholarship Outstanding students (October Evaluation of 2024) Outstanding Student cadres (October Evaluation of 2023) Outstanding Student Award in the School of Information Engineering and Science Top 10 Students• Courses: Engineering Physics, Introduction to the Physics of Semiconductors, Electrodynamics, AI Enhanced Simulations.		

PUBLICATION

ZiJie Qiu,1, * Luozhijie Jin,2, * Zijian Du,3 Hongyu Chen,2, 4 **Guanyao Mao**,2, 4 Yan Cen,3, † Siqi Sun,1 Yongfeng Mei,5 and Hao Zhang2, 4, 6, ‡. VQCrystal: Leveraging Vector Quantization on Large-scale Discovery of Crystal Structures across Dimensionalities (Nature Parter Journal Public 2025)

Guanyao Mao, Zhiyang Dou, Minghao Guo, Benjamin Tod Jones, Wojciech Matusik AutoAxiom: Automated Axiom Modification for Scientific Discovery with LLMs. (To be submitted ICML 2026)

Zijian Du,1, 2, * Luozhijie Jin,1, * **Guanyao Mao**,1 Hongyu Chen,1 Yan Cen,2, † Yongfeng Mei,3 and Hao Zhang1, 4, 5, ‡. CTGNN: Crystal Transformer Graph Neural Network for Crystal Material Property Prediction (Preprint 2025)

Chinese Invention Patent (pending): “Concentrated photovoltaic-thermoelectric hybrid power generation device and method” Application No. 202410987613.3 (**first inventor among undergraduates**)

RESEARCH EXPERIENCE

ZhangLab (Fudan University)	Shanghai, China	
		03/2023-07/2025
<i>Research Assistant, Advisor: Prof. Hao Zhang</i>		
<ul style="list-style-type: none">• My research leverages DFT tools like VASP and ShengBTE to explore the unique properties of the topological material Te. Through Electron-Phonon-Wannier calculations, I've found that SOC significantly impacts phonon scattering between Te's CBM and VBM. Additionally, Te's thermal conductivity decreases with increasing crystal layers.• I've contributed to developing CTUAE and CTGNN—algorithms that predict crystal structures with enhanced accuracy in material properties like formation energy. Additionally, I participated in creating PARCE, an algorithm that generates crystal structures from compound Raman spectra, showcasing the potential of ML in crystal creation.• To tackle the efficiency limitations in transforming solar energy into electricity in polar cells, I designed an integrated system that combines Fresnel light concentration with the utilization of thermal energy generated		

by solar cells. By incorporating thermoelectric materials to convert this heat into electricity, I achieved a significant increase in the energy conversion efficiency of our cells, from 25% to 38%.

- Large Language Models (LLMs) hold immense potential for scientific discoveries. I integrated Retrieval-Augmented Generation (RAG) into thermoelectric materials research by embedding over 2,000 documents into the LLM. Addressing the challenge of benchmarking LLMs in AI for Science, I developed a novel multiple-choice examination system to assess their accuracy. Applying this to GPT-4o-min, I observed a nearly 15% improvement in accuracy for materials science tasks.

MIT CDFG (MIT EECS)

Cambridge, MA 02139

08/2025 - Present

Research Assistant, Advisor: Prof. Wojciech Matusik

- Developed AutoAxiom, a neuro-symbolic framework combining LLMs with physics-based symbolic reasoning for automated scientific law discovery. Enables autonomous axiom evolution, multi-agent validation of axiom performance, and seamless extension to diverse domains, unlocking LLMs' potential to revolutionize engineering decisions and scientific discovery.
- I designed and implemented a dual-layer language system (minimalist AxiomDSL + rigorous AxiomIR), enabling humans to define scientific laws in a few natural lines while allowing LLMs to precisely and safely edit every single expression leaf. Under zero-trust toward LLMs, it fully unleashes their creativity and achieves genuine closed-loop automated scientific discovery.

OTHER EXPERIENCE

Mathematical Contest In Modeling 2024

Kunming, China

Team Leader & Participant

02/2024

- As the team leader and paper supervisor, established a submarine search and rescue model based on Bayesian optimization.
- Honor : H prize for the MCM of 2024

National College Students Internet Plus Innovation and Entrepreneurship Competition 2025

Shanghai

Team Leader & Project Leader

- As the team leader and project supervisor, developed a Concentrated-Photovoltaic-Thermoelectric (CPV-TE) hybrid cell system integrating Fresnel light concentration and thermoelectric materials to enhance solar energy conversion efficiency.
- Award: Silver Prize in Shanghai Municipal Division for the 2024 Internet Plus Competition

SKILLS & HOBBIES

- **Skills:** Familiar with DFT software such as vasp, tdep, phonopy, quantum espresso; office software such as Overleaf, Powerpoints, Ai Illustrator; programming languages such as python; artificial intelligence agent building technologies such as Fine Tune, RAG, openvino, pytorch, and physical simulation etc.
- **Standardized Tests:** TOEFL (All scores best): 104 (R: 30 L: 28 S: 23 W: 23) and 102(Single) (R: 29 L: 28 S: 23 W: 22)
- **Hobbies:** Playing the drums (Drum set, Grade: 9), Tennis (School-level competition bronze medal) . Middle and long-distance running(National Level 2 Marathon Athlete, Gold medal in the 5000-meter inter-school sports meet) Table Tennis(Silver medal in college competition)