

Guanyao Mao
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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, †} Siqu Sun,¹ Yongfeng Mei,⁵ and Hao Zhang^{2, 4, 6, ‡}. VQCrystal: Leveraging Vector Quantization on Large-scale Discovery of Crystal Structures across Dimensionalities (Nature Partner 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 Zhang^{1, 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

Research Assistant, Advisor: Prof. Hao Zhang

- 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)