

Guoyue Xu

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Professional Summary

- **PhD candidate in Mechanical Engineering** with expertise in **AI for Science (AI4S)**, focusing on LLM multi-agent systems, autonomous scientific discovery, and Bayesian optimization
- **Proven impact:** Developed self-driving laboratory pipelines that improved polymer discovery efficiency by **5x** and engineered Bayesian optimization frameworks reducing experiments by **80%**
- **Expertise:** LLM multi-agent orchestration, scientific reasoning agents, Bayesian optimization, computer vision, and probabilistic models

Education

- 2023–Present **PhD in Mechanical Engineering**, *University of Notre Dame*, Notre Dame, IN
Focus: Machine Learning for Materials Discovery, Bayesian Optimization, Neural Networks
- 2021–2023 **MS in Electrical Engineering**, *University of Notre Dame*, Notre Dame, IN
- 2016–2020 **BSc in Communications Engineering**, *National Chung Cheng University*, Taiwan, **GPA:** 3.83/4.3 (Top 3)
Honors: President Scholarship (Top 2%), Director Scholarship (Top 5%)

Publications & Preprints

- 2025 Xu, G.*, Zhang, R., & Luo, T. "Self-Driving Laboratory Optimizes the Lower Critical Solution Temperature of Thermoresponsive Polymers." *arXiv preprint arXiv:2509.05351* (2025).
- 2025 Zhang, R.*, Xu, J., Zhang, H., Xu, G., & Luo, T. "Active learning-guided exploration of thermally conductive polymers under strain." *Digital Discovery*, 4(3), 812–823 (2025).
- 2024 Pan, Z.*, Xia, J., Yan, Z., Xu, G., et al. "Rethinking Medical Anomaly Detection in Brain MRI: An Image Quality Assessment Perspective." *arXiv preprint arXiv:2408.08228* (2024).
- 2024 Song, K.*, Xu, G.* , et al. "Machine Learning-Assisted 3D Printing of Thermoelectric Materials." *Journal of Materials Chemistry A*.
- 2020 Xu, G.* , et al. "Harvesting Electromagnetic Energy in Air: A Wireless Energy Harvester at 2.45 GHz." *IEEE Microwave Magazine*, 21(6), 88–95 (2020).

Research & AI4Science Projects

- 2025–Present **LLM Multi-Agent System for Polymer Thermal Conductivity (TC-CoScientist)**, *Notre Dame*
 - Designed an LLM-powered orchestration agent to autonomously manage polymer thermal conductivity discovery.
 - Integrated molecular dynamics simulations, graph neural networks, and interpretable reasoning into a closed-loop self-driving discovery workflow.
- 2025–Present **Vision Language Model for Laboratory Experiment Understanding**, *Notre Dame*
 - Developed a protocol-guided VLA model to align experimental SOPs with lab figures.
 - Contributed to emerging AI4Science efforts in scientific experiment understanding.

- 2023–Present **Autonomous Materials Discovery System (Self-driving labs)**, *University of Notre Dame*
- Designed and built a low-cost, Arduino-based self-driving laboratory for autonomous polymer and thermo-responsive optimization.
 - Integrated robotic fluid handling PID-controlled thermoelectric heating/cooling and in-situ optical sensing.
 - Implemented a closed-loop Bayesian optimization pipeline using Gaussian Process Regression (GPR) to autonomously explore multi-component chemical spaces.
 - Achieved reproducible, self-correcting optimization of thermoresponsive polymer LCST while reducing experimental requirements by **80%**.
- 2024 **Medical Anomaly Detection in Brain MRI**, *University of Notre Dame*
- Developed a novel image quality assessment (IQA) framework for medical anomaly detection in brain MRI scans, reframing anomaly detection as an image quality problem to improve diagnostic accuracy.
 - Implemented deep learning models combining convolutional neural networks with quality assessment metrics, achieving state-of-the-art performance on multiple brain MRI datasets.
 - Built comprehensive evaluation pipeline with multiple benchmark datasets, demonstrating superior performance over traditional anomaly detection methods in medical imaging.
- 2024 **GAN-based Text Generation**, *University of Notre Dame*
- Designed a four-layer generative adversarial network (GAN) architecture for text generation and stabilised training using LeakyReLU activations and gradient penalty regularization.
 - Implemented beam search and temperature scaling decoders for GPT-2 embeddings, increasing text quality and diversity as measured by BLEU scores and t-SNE visualization.
 - Built a comprehensive evaluation framework incorporating BLEU scores, t-SNE plots and qualitative assessments to benchmark against baseline models.

Research & Engineering Experience

- 2021–2022 **Signal Processing & SDR Systems Engineer**, *University of Notre Dame*, Notre Dame, IN
- Designed and implemented a **software-defined radio (SDR) communication system** for hands-on instruction and research
 - Built a progressive learning and prototyping framework that transitioned from wired transmission models to full wireless implementations, addressing propagation, interference, and noise challenges in congested RF environments.
 - Developed an automated Python/C-based control and data acquisition pipeline for real-time signal testing and debugging, reducing manual workload by **70%** and improving system throughput.
- 2019–2020 **Project Lead & RF Engineer**, *National Chung Cheng University*, Taiwan
- Led a team to **1st place** in the 2019 IEEE MTT-S Student Design Competition by developing a wearable microwave energy harvester.
 - Designed and simulated a high-performance patch antenna with a **24.4 dB** return loss at 2.45 GHz and **5.18 dB** maximum gain using HFSS.
 - Engineered a $50\ \Omega$ matched rectifier circuit with Schottky diodes, achieving high RF-to-DC conversion efficiency and validating performance through VNA analysis.

Awards & Recognition

- 2019–2021 **President Scholarship** (Top 2%) & **Director Scholarship** (Top 5%, 2×) – National Chung Cheng University
- 2020 **Professor Chun-Hsiung Chen Scholarship** – Academic Excellence Recognition
- 2019 **1st Place Winner** – IEEE Microwave Theory and Techniques Society Student Design Competition

Technical Skills

- Programming **Python**: PyTorch, TensorFlow, Scikit-learn, NumPy, Pandas, Matplotlib, Jupyter
- Machine Learning **Deep Learning**: CNNs, GANs, Transformers, Bayesian Optimization, Gaussian Processes, Active Learning
- AI4Science **LLM & Multi-Agent Systems**: Scientific reasoning agents, autonomous orchestration, tool-augmented LLMs
- Electrical Engineering **RF & Microwave**: Antenna design (HFSS, CST), RF energy harvesting, impedance matching, rectifier circuits, VNA characterization, Advanced Design System (ADS)