

Lavudya Akhil

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Education

B.Tech, Indian Institute of Technology Guwahati, India

2023 - Ongoing

Major in Chemical Science and Technology

Experience

Chemistry, Manufacturing, and Controls (CMC) Lab

IIT Guwahati, India

MATERIA — Agentic AI Platform for Materials Simulation

May 2026 – Jun 2026

AI/ML Research Intern

[Github](#) 

- Built an agentic AI platform (26K LOC; FastAPI + React) driven by a 23-tool Gemini function-calling agent that converts natural-language prompts into real materials-science simulations (DFT input generation + ML-potential physics).
- Benchmarked 6 pretrained ML interatomic potentials (MACE, MatterSim) against Materials Project DFT across 60 relaxations, achieving 2.65% mean volume error via an end-to-end EOS-fitting and parity-analysis pipeline.
- Validated 100% tool-selection and argument accuracy across a 39-prompt suite at 2.09 s mean latency.
- Engineered async compute (Celery/Redis + PostgreSQL) with JWT + Fernet-encrypted key storage and a Gemini→Ollama failover chain.

DKL-BO — Deep Kernel Learning + Bayesian Optimization

Jun 2026 – Jul 2026

AI/ML Research Intern

[Github](#) 

- Designed from scratch a Deep Kernel Learning surrogate (CGCNN encoder + Gaussian Process, jointly trained) for Bayesian optimization over a 3,351-material space, locating the global optimum within ~3% of evaluations — $6.3\times$ more sample-efficient than random search.
- Ran a controlled 30-seed study with paired Wilcoxon tests ($p\approx 0.002$) isolating pre-training data size as the variable governing when deep-kernel representations beat handcrafted descriptors (crossover at $N\approx 250-500$).
- Calibrated surrogate uncertainty (temperature scaling + isotonic recalibration) to Coverage@95 = 0.93 (MAE 0.45 eV).
- Built an LMDB graph cache cutting ~3,000 redundant GNN passes per BO cycle; first-author manuscript in preparation.

Projects

Sage — Agentic Multi-Tool RAG Chatbot

Apr 2026

Personal Project

[Live Demo](#) 

- Built an agentic LLM chatbot — a LangGraph conditional tool-execution graph routing a Groq Llama-3.1-8B model across 4 tools (web search, finance API, calculator, PDF retrieval) with token streaming.
- Implemented per-document RAG over uploaded PDFs (all-MiniLM-L6-v2 embeddings + Qdrant per-thread filter), scoring 100% hit-rate@4 / 1.000 MRR on a 13-question evaluation harness.
- Deployed a thin Streamlit client over a serverless Modal FastAPI backend (scales to zero), with persistent multi-thread memory via a Neon Postgres checkpointer and LangSmith tracing.

NFL Draft Prediction — GCI World 2026 (Top 10% Worldwide)

Jun 2026

GCI Competition

[Github](#) 

- Built a LightGBM + CatBoost ensemble (Optuna-tuned over 50 trials, 5-fold stratified CV, 3-seed averaging) reaching 0.829 OOF ROC AUC on 2,781 combine records — ~ 0.05 AUC over baseline.
- Engineered missingness-as-signal features (a single missing-age flag alone $\rightarrow$ 0.716 AUC) and leak-safe fold-internal target encoding with Bayesian smoothing, validated leak-free on out-of-fold predictions.
- Packaged into a tested, pip-installable module and deployed the ensemble as a serverless Modal `/predict` API with a Gradio UI and SHAP per-prediction explanations.

Technical Skills

- Core: Machine Learning, Deep Learning
- Frameworks: PyTorch, TensorFlow, Keras, scikit-learn, LangChain, LangGraph, OpenCV
- Front-End: HTML, CSS, JavaScript, React.js, Next.js
- Databases: PostgreSQL, MySQL, Qdrant, Neon
- Tools: Git, GitHub, LangSmith
- Programming: Python, SQL, C/C++
- Libraries: Pandas, NumPy, Matplotlib, Seaborn, Power BI, LightGBM, CatBoost, Optuna
- Back-End: Node.js, Express.js, FastAPI, Celery/Redis
- Deployment: Docker, AWS, Modal, Streamlit

Achievements

- Codeforces: Solved 350+ problems [Akhil31_07](#) 
- LeetCode: Solved 200+ problems [akhil31_07](#) 
- GCI World 2026 data-science competition — Top 10% worldwide (NFL Draft Prediction)
- JEE Main & JEE Advanced 2022: Cleared both of India's most competitive engineering entrance exams — among the top 0.15 million out of over 1 million candidates nationwide
- Gold Medals, Spardha Inter-Hostel Sports (Kabaddi 2024 & 2026, Hockey 2025), IIT Guwahati