Satnam Singh

AI/ML Research: Materials Science, Language Models, and High-Performance Computing

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Research Interests

Machine learning applied to physical and materials systems, including graph neural networks for defect prediction. Also interested in retrieval-augmented language model systems and GPU-accelerated computing for training and inference at scale.

Education

Christ University, Bengaluru, India 05/2025 – 06/2029
B.Tech in Computer Science and Engineering (AI and ML). CGPA: 3.79/4.0 (First Year)

Indian Institute of Technology Madras, India 07/2025 – 07/2029
B.S. in Data Science and Applications (Online, concurrent degree)

Research Experience

Graph Neural Networks for Defect-Site-Resolved p-type Dopant Viability in β-Ga_2O_3 08/2026 – Present
Centre of Excellence for Frontier Materials Research, Christ University, Bangalore

- Designing a defect-site-resolved graph representation encoding dopant identity, substitutional site, coordination geometry, and formal charge state as node and edge attributes, to predict defect formation energy and ionization level directly from doped crystal structures.
- Training and validating on a public DFT-derived dataset of approximately 15,000 defect structures across roughly 40 zinc-blende compounds, with planned benchmarking against random forest and gradient-boosted baselines.
- Targeting five divalent acceptor dopants at both inequivalent Ga sites of β-Ga_2O_3, toward an interpretable p-type viability ranking. Abstract under review at the 80th Annual Technical Meeting of the Indian Institute of Metals (IIM ATM 2026) and the International Symposium on Materials for Sustainable, Green and Nuclear Energy Applications, BISR, Jaipur.

Applied Machine Learning Projects

NodeGuard – Graph Neural Network for Financial Fraud Ring Detection 09/2026
PyTorch Geometric, Python

- Designed a 2-layer graph convolutional network to detect coordinated fraud rings from transaction-network structure rather than isolated account features, modeling two anti-money-laundering typologies under severe class imbalance.
- Identified and corrected a validation-metric selection flaw (recall-only checkpointing converging on a degenerate solution) with F1-based checkpointing; built a reproducible evaluation pipeline.

Domain-Specific Retrieval-Augmented Generation System 08/2026 – Present
Python, LangGraph, FAISS

- Built a multi-agent retrieval pipeline over a scientific literature corpus with sentence-level natural language inference verification of generated claims against retrieved evidence.

HPC and GPU Programming

Custom CUDA Matrix Multiplication Kernels 05/2026 – Present
CUDA, C++, C

- Writing custom CUDA SGEMM kernels toward cuBLAS-class performance, progressing from naive GEMM to coalesced global-memory access and shared-memory tiled designs; improved FP32 throughput from 169.6 to 1052.9 GFLOPS on an RTX 4060, a 6.5x speedup, through warp-aware thread mapping and 32x32 shared-memory tiling.
- Profiling and validating correctness with CUDA events, Nsight Systems, Nsight Compute, and ptxas; extending the work with register blocking, warp tiling, and Tensor Core / WMMA paths.

Other Technical Projects

RISC-V Database System 06/2026
PostgreSQL, Python, YAML, JSON

- Built a Python ETL pipeline extracting RISC-V's official ISA specification from 1,700+ YAML files into a normalized PostgreSQL database with enforced referential integrity across 8 relational tables, covering 1,351 instructions and 396 control/status registers.

Skills

Languages: Python, C++, C, SQL **Tools:** CUDA, FastAPI, Docker, Git, Linux, PostgreSQL
ML/DL Frameworks: PyTorch, PyTorch Geometric, XGBoost, Scikit-learn, LangGraph, FAISS