

Vani Nigam

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Education

Carnegie Mellon University, Pittsburgh, PA, United States of America

Master's in Artificial Intelligence in Materials Engineering

December 2026

Selected Coursework: Systems and Tool Chains, Machine Learning for Engineers, Generative AI, Introduction to Deep Learning

Indian Institute of Technology [IIT], Bhubaneswar, Odisha, India

Bachelor's in Metallurgy and Materials Engineering, GPA: 8.20/10.0

April 2025

Selected Coursework: Numerical Methods, Introduction to Simulation and Modelling, International Business, Intro to Economics, Industrial Manufacturing, Corrosion and Surface Engineering, Elements of Electroceramics.

Skills

Libraries: Pandas, NumPy, Matplotlib, Keras, spaCy, Scikit, Tensorflow, LangChain, Pytorch

Models: DeepChem, BERT, BigSMILES, ChemBERTa, HuggingFace Transformers, LSTM, ElasticNet

Tools: Python, SQL, Docker, LAMMPS, MATLAB, Power BI, Streamlit, Gradio

MLOps & Scalability: Neo4j, PySpark, Kafka, MosaicML, Model Context Protocol

Internship

Summer Research Intern

Department of Energy Science, Indian Institute of Technology, Bombay, India

May 2024 –July 2024

- Conducted scientometric analysis of research articles using Python and R software, like BibExcel and VOSviewer, and ML library SpaCy for extracting the highest cited work in the advancements of catalysts being researched worldwide.
- Developed statistical indices to visualize progress in 6,000+ papers on Magnesium-based alloys in solid-state Hydrogen storage systems and conducted comparative analysis on the grounds of the catalyst class, using Regex for sequences.

Projects

Agent Orchestration for Polymer Property Prediction

Master's Project, Mechanical and AI Lab

September 2025 – Present

- Designed an intelligent polymer AI Agent integrating LLMs for natural language query parsing with the TransPolymer, a pretrained transformer model for SMILES sequence sanity checking, and iterative modification by leveraging FastMCP server and finetuned Molecule Chef (2019) for suggesting candidate polymers.
- Enabled automated prediction of polymer properties (bandgap, conductivity, dielectric constant, etc.) directly from polymer SMILES vector representations, and further modification of the polymer structure according to the user query.

Thoughts-Trader Psychologically aware conversationalist AI Agent

Voluntary Research Position, Human-Computer Interaction Center (HCI)

September 2025 – Present

- Orchestrated a conversational AI (CAI) model by developing a LangChain-based RAG architecture to efficiently prompt the GPT API to shift role according to the psychologically nuanced responses of the user.
- Worked with the Machine Learning team to deploy the CAI service to integrate the chat API to ensure scalable, real-time performance and seamless data flow in a physical robotic system for users to converse with the AI agent during nighttime.

Time Series Classification with Deterministic Learning

Bachelor's Thesis Project, Professor Brahma Deo, India

April 2024 – April 2025

- Constructed an RBF Neural Network for EEG classification, emphasizing feature extraction and strategic handling of imbalanced data; the model was trained in over 2,000 time-series samples, ensuring consistent predictions.
- Analyzed the wavelet decompositions using the Discrete Wavelet Transform to reconstruct the EEG data and fit into the Entropy measures for feature extraction, to train the Neural Network, and increase efficiency to 72% from 50%.

Publications

- 'A Confluence of Emerging Technologies : IoT, Edge, and Cloud Computing, Blockchain, Industry 4.0 and 5.0, AI and ML toward the Realization of Eco-Friendly Supercapacitors.' Vinay Katari, Samarthya Goyal, **Vani Nigam**, Milan Jana, Anirban Maitra, Henu Sharma, and Kisor K. Sahu (2025), American Chemical Society