Vani Nigam

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Educations

Carnegie Mellon University, Pittsburgh, PA, USA
Master's in Artificial Intelligence in Materials Engineering   *2025-2026*
Courses: *Systems and Tool Chains for AI, Machine Learning for Engineers, Foundations of Materials Science, Trustworthy AI, Computational Material Science.*

Indian Institute of Technology [IIT], Bhubaneswar, Odisha, India   GPA: 8.20/10.0
Bachelor's in Metallurgy and Materials Engineering   *2021-2025*
Courses: Numerical Methods, Introduction to Simulation and Modelling, Corrosion and Surface Engineering, Elements of Electroceramics, Chaos and Dynamical Systems.

Technical Skills

Libraries: Pandas, NumPy, Matplotlib, Keras, spaCy, Streamlit, Gradio, Scikit, Tensorflow, LangChain
Models: Rdkit, Scikitmol, DeepChem, BERT, BigSMILES, ChemBERTa, HuggingFace Transformers
Tools: Python, SQL,Docker, MATLAB, Power BI,LAMMPS, ThermoCalc, Vantage Point v16.0, MS Excel

Internship Experience

Department of Energy Science, IIT Bombay, India | Research Intern   *May 2024 – July 2024*
• Scientometric analysis of hydrogen studies using Python and R software, like BibExcel and VOSviewer, for extracting information for a qualitative study of 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 diverse grounds.

Projects

Polymer Property Prediction via Multimodal Learning | Github Link
• Designed a multimodal ML pipeline combining SMILES-based LSTM encoders and Morgan fingerprint vectors (RDKit, ScikitMol) to predict polymer properties (e.g., FFV, Tg, Tc).
• Implemented domain-specific feature extraction using Morgan fingerprints, descriptor vectors, and SELFIES-based tokenization; stored embeddings and tensors for efficient training, using custom weighted-MAE loss.

Time Series Classification with Deterministic Learning | Bachelor's Project under Prof. Brahma Deo
• Constructed an RBF Neural Network for EEG classification, emphasizing feature extraction and strategic handling of imbalanced data; the model was trained over 2,000 time-series samples, ensuring consistent predictions.
• Analysed the wavelet decompositions using Discrete Wavelet Transform to reconstruct the wavelets using the wavelet package and fit into the Entropy measures for feature extraction, to train the Neural Network, and increase efficiency.

Battery Life Prediction (Dr. Kisore Sahu and Electrogati Ltd., Hyderabad) | Github Link
• Explored data analysis techniques for predicting Li-ion battery life by handling feature engineering from the data obtained from 124 Li-ion cells to visualize the feature representation in a compact basis.
• Used the data from Lithium Ion Phosphate batteries using Matplotlib to plot voltage cycles, discharge curves, etc. to obtain interpretable statistical inferences and predict early insights before degradation.

Publications

Kisor et al , 2024 Book Chapter Co-Authorship , American Chemical Society
• 'A Confluence of Emerging Technologies Like IoT, Edge, and Cloud Computing, Blockchain, Industry 4.0 and 5.0, AI and ML toward the Realization of Eco-Friendly Supercapacitors.'
• Analyzed articles on Cloud Computing and Edge Computing for working towards the realization of green supercapacitors in the industry.

Leadership

• Student Placement Coordinator, Career Development Cell, IIT Bhubaneswar, India   2024 -2025
• Governor, English Literary Society, Gymkhana Council, IIT Bhubaneswar , India   2023 - 2025