Dominic Varghese

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Professional Summary

Computational Ph.D. candidate (Materials Science, UMN) with expertise in machine learning, scientific computing, and fundamental R&D. My work focuses on building and applying complex predictive models - from first principles simulations (DFT, MD) to AI-driven algorithms using PyTorch and Scikit-learn. I am proficient in Python and C and experienced in GPU-accelerated HPC environments, with a technical focus on accelerating materials discovery.

Skills

Technical Skills: First-principles calculations (DFT, DFPT) , Molecular Dynamics , High Performance Computing

Frameworks: VASP , ABINIT , Quantum Espresso , LAMMPS

Languages: Python , C , Git , Bash , HTML , CSS

Machine Learning: PyTorch , NLTK , Scikit-learn , Pandas , Numpy

Research Experience

Flexoelectric effect in binary metal oxides — Graduate Research Assistant

Advisor: Prof. Turan Birol CEMS, University of Minnesota — *Dec 2023 - Present*

- Fine-tuning foundational Machine Learning Interatomic Potentials (MLIPs) to enable accurate and efficient modeling of flexoelectricity in larger, more complex crystal structures.
- Discovered that epitaxial strain significantly enhances the flexoelectric coefficient in alkaline-earth-metal oxides by lowering optical phonon mode frequencies.
- Quantified the relationship between strain and flexoelectric tensor components using first-principles calculations (DFT, DFPT), Landau theory, and Group theory.
- Build a high-efficiency, scalable simulation framework, enabling the accurate modeling of flexoelectricity in larger, more complex crystal structures that are inaccessible to traditional DFT.

Non-linear Hall effect in Ferroelectrics — Undergraduate Researcher

Advisor: Prof. Awadhesh Narayan SSCU, Indian Institute of Science — *Aug 2022 - Jun 2023*

- Identified optimal doping concentrations in ferroelectric perovskites that maximize the Berry Curvature Dipole (BCD), leading to an enhancement of the Non-Linear Hall effect.
- Systematically varied doping concentrations and computed BCD using Quantum Espresso and Wannier90, successfully demonstrating a tunable electronic response.

Machine Learning Projects

Fraud Detection in Financial Transactions Using Machine Learning — *Fall 2024*

- Engineered and evaluated multiple classifiers: K-Means Clustering, SVM, Naive Bayes to detect fraud within a highly imbalanced dataset of 1 million transactions.
- Optimized a SVM with an RBF kernel, achieving a robust AUC of 0.93 and capturing 69% of fraudulent cases at a practical 5% False Positive Rate.
- Constructed a K-Means clustering pipeline using Random Under-Sampling and PCA to overcome class imbalance, boosting model performance to a peak F1-score of 0.80.

Piezoelectric Modulus Prediction Using Machine Learning — *Spring 2024*

- Developed an innovative data science pipeline to predict the piezoelectric modulus for 1,354 unique inorganic materials from the JARVIS database.
- Achieved 78% accuracy with an XGBoost classifier to identify piezoelectric materials, utilizing SHAP analysis to discover that crystal symmetry was a critical predictive feature.
- Tuned a LightGBM regression model that accurately predicted piezoelectric constants, achieving a final Root Mean Squared Error of 0.49 by integrating a pre-trained model for band gap prediction.

Predicting Band Gap in Inorganic Materials Using Machine Learning — *Spring 2023*

- Explored 4 ML algorithms - regression, SVM, decision trees and neural networks - to create a predictive framework for inorganic material band gaps.
- Built a classification pipeline that successfully categorized materials as conductors or insulators, identifying XGBoost as the most accurate and efficient model for the task.
- Demonstrated that Artificial Neural Networks outperformed all other tested models for the regression task, establishing them as the superior method for predicting precise band gap values.

Education

University of Minnesota — Twin-Cities, US
Doctor of Philosophy - Materials Science; CGPA 3.8/4 — *Sep 2023 - 2028*

Indian Institute of Science — Bengaluru, India
Master of Science - Chemistry; CGPA 8.8/10 — *Aug 2022 - Jul 2023*

Indian Institute of Science — Bengaluru, India
Bachelor of Science Research - Chemistry (Major) and Materials (Minor); CGPA 8.6/10 — *Aug 2018 - Jul 2022*

Publications

Flexoelectric effect in alkaline earth metal oxides; Dominic Varghese, et al.: *Manuscript under preparation*

Berry Curvature Dipole in Ferroelectrics; Dominic Varghese, et al.: *Manuscript under preparation*

Growth of Co_9S_8 Islands on Cu_2S Nano-Disks; Biman Jana, Dominic Varghese, Awadhesh Narayan, Anshu Pandey: *J. Phys. Chem. C 2023, 127, 18, 88738879*

Cobalt(I)-Catalyzed Borylation of Unactivated Alkyl Bromides and Chlorides; Piyush K. Verma, K. Sujit Prasad, Dominic Varghese, K. Geetharani: *Org. Lett., 2020, 22, 1431-1436*

Honors

NSF ACCESS Discover Grant (2025 - 2026)
Recipient of a resource allocation grant from the National Science Foundation (NSF) for access to the nation's advanced high-performance computing systems.

Oral Presentation at APS Global Summit 2025, Anaheim, CA
Presented doctoral research on the Flexoelectric Effect in Binary Metal Oxides.

Poster Presentation at Ferroelectric Oxides Materials and Devices Conference 2023 at Bengaluru, India
Presented Master's thesis research on the Non-Linear Hall Effect in ferroelectrics.

Kishore Vaigyanik Protsahan Yojana (KVPY) Fellowship (2018 - 2023)
Awarded by the Government of India for exceptional promise in scientific research.

Teaching Experience

Teaching Assistant, MatS 4301: Materials Processing — *Spring 2024*
Led laboratory sessions for 25 final-year undergraduate students, demonstrating key materials processing techniques including X-Ray Diffraction, Sputtering, Dip Coating, etc.