Pravan Omprakash

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PhD candidate in Materials Science with expertise in **Atomistic modelling** and **Data-driven modelling**. Experienced in building **Python** tools for large-scale materials discovery using **Density Functional Theory**. Interested in applying **ML** and **statistical analysis** to solve complex data-driven problems.

Education

2023 - PhD candidate from **Washington University in St Louis, USA** (GPA: 3.75/4)
2018 - 2022 BTech from **National Institute of Technology, Karnataka, India** (GPA: 3.6/4)

Research Experience

PhD Candidate @ MCUBE Lab, WashU Jan 2023 - present

Develop methods to accelerate alloy discovery of High Entropy Alloys using a mix of Density Functional Theory, Classical Thermodynamics and ML, under the guidance of Dr. Rohan Mishra. Provide theoretical support for experimental observations in polar materials like hexagonal manganites and ZrO_2.

Undergraduate Research Jan 2019 - July 2022

- Worked with Dr. Kisor Kumar Sahu and Dr. Swayamjyoti S at IIT-Bhubaneshwar to develop ML models for inverse design of metamaterials and vibration-based energy harvesters.
- Contributed to developing a U-NET based segmentation model for detecting lung X-ray image opacities with Dr Avantika Vardhan at Feinstein Institutes for Medical Research.

Selected Projects

Exploring the interplay of disorder and order in materials

→ **Visualizing high-dimensional spaces using SymPlex plots** • Publication @ Scripta Materialia • Presentation @ MRS Fall'25 **(Awarded Best Oral Presentation)** • Code @

→ **Rapid phase diagram prediction of multinary alloys** • Presentation @ MRS Fall'25 & TMS'26 • Poster @ NASSCC'25

Investigating ferroelectricity in Hafnia

→ **Hole Doping lowers the coercive field of Hafnia** • Preprint @ Arxiv • Poster @ Ferro'24

→ **Antiferroelectric Phase Stabilization at 2D limit in Hafnia** • Preprint @ Arxiv (Revision in Science)

Developing ML models for various applications

→ **Graph Neural Networks for material property prediction** • Publication @ Computational Materials Science • Code @

→ **CNN for facial movement recognition** • Presentation @ AAAI'21 **(Top 20 student abstracts)** • Code @

Technical Skills

Programming Python, NumPy, Pandas, SciPy, Matplotlib, Plotly
Machine Learning PyTorch, TensorFlow, Scikit-learn
Computational Materials Science Density Functional Theory (VASP), Molecular Dynamics (LAMMPS), Pymatgen