Pravan Omprakash

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I am pursuing a **PhD in Materials Science**, wherein I explore the interplay of disorder and order in complex materials ranging from metallic alloys to polar semiconductors, using **density functional theory, thermodynamic models and data science**. I collaborate with various experimental groups to guide material design and provide theoretical support. I am excited to use ML to investigate physical phenomena, and push the frontier of materials design.

Education

2023 - Material Science PhD from **Washington University at 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

I develop methods to rapidly predict alloy phase diagrams of multinary materials using a mix of Density Functional Theory, Classical Thermodynamics and ML, under the guidance of Dr. Rohan Mishra. I also provide theoretical support for experimental observations in polar materials like hexagonal manganites and ZrO_2.

Undergraduate Research Jan 2019 - July 2022

- I worked with Dr. Kisor Kumar Sahu and Dr. Swayamjyoti S at IIT-Bhubaneshwar to develop machine learning models for inverse design of metamaterials and vibration-based energy harvesters.
- I 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 Publications

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

Developing ML models for various applications

→ **Graph Neural Networks** • Publication @ Computational Materials Science • Code @

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

Skills

Coding packages	Python, PyTorch, Tensorflow
Computational Materials Science packages	VASP, LAMMPS