Pravan Omprakash

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Summary

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 experimental groups to guide design and provide theoretical support. I am excited to use ML to investigate physical phenomena, especially to 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 research high entropy alloys and develop methods to rapidly predict phase diagrams of multinary materials using a mix of Quantum Mechanics, Classical Thermodynamics and Machine Learning. I also provide theoretical support for experimental observations in polar materials.

Undergraduate Research Jan 2019 - July 2022

- I collaborated with professors and students at NITK, Surathkal on diverse projects including developing graph and convolution neural networks for various applications as well as reviewing the progress of nanomaterials for electronic devices.
- I worked with Prof. 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 •Poster @ TMS'26 •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 (Contributing author)
- **Atomically thin charged domain walls in zirconia** •Preprint @ Arxiv (Contributing author)

Developing ML models for various applications

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

- **GAN for Inverse Design of Metamaterials** •Presentation @ WCCM'22
- **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