Yagnik Bandyopadhyay

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SUMMARY

PhD researcher working at the intersection of machine learning, quantum-mechanical simulation, and data-driven models for complex physical systems. Experience applying deep learning, generative models, and physics-informed AI to real-world scientific and energy-related problems.

EDUCATION

PhD, Mechanical Engineering **May 2027 (expected)**
Arizona State University, Tempe, AZ 3.75 GPA
Ira A. Fulton Schools of Engineering
Relevant coursework: Applied Machine Learning for Mechanical Engineers, Quantum Mechanics, Applied Linear Algebra

MS, Aerospace Engineering **May 2023**
Arizona State University, Tempe, AZ 3.75 GPA
Ira A. Fulton Schools of Engineering
Relevant coursework: Finite Element Methods, High Performance Computing, Linear Algebra, Partial Differential Equations, Advanced Numerical Method for PDEs]

TECHNICAL SKILLS

Programming: Python, Matlab, Fortran
Simulation Package: Vienna Ab-Initio Simulation Package (VASP), LAMMPS, hiPhive
Frameworks and Libraries: PyTorch, TensorFlow, Scikit-learn, Keras, Qiskit
Data Analysis Libraries: Pandas, Numpy
Design/ Visualization Software: Vesta, Solid Works, Creo, ANSYS, Abaqus

RESEARCH EXPERIENCE

IPAM, UCLA – Visiting Researcher Aug 2025 – Dec 2025
Los Angeles, CA

- Conducted research on generative AI (autoregressive and diffusion models) for data-driven modeling and decision-support in physical and energy-relevant systems, with emphasis on uncertainty, stability, and physical feasibility.
- Validated AI-generated water structures using RDFs, geometric statistics, and energy analysis, benchmarking against MD data.
- Proposed physics-guided and conditional generative modeling to improve stability and chemical realism.

ACADEMIC PROJECTS

Large Language Models for Thermoelectric Materials Discovery Spring 2025 - Present
Developing LLM-based regression and representation learning pipelines for energy-relevant materials modeling.

- Developed LLM-based models to predict thermoelectric performance (e.g., ZT) from composition and temperature-dependent descriptors.
- Designed structured input representations and prompt-based workflows to integrate domain knowledge into LLM-assisted regression tasks.
- Benchmarked LLM predictions against classical machine learning baselines (ANNs, tree-based models) to assess generalization and uncertainty.
- Analyzed model performance using statistical metrics and error diagnostics to identify physically inconsistent predictions.
- Ongoing research project; manuscript in preparation.

Predicting Baseball Game Outcomes Using Machine Learning November 2023
Applied supervised machine learning models to real-world, noisy outcome prediction problems.

- Developed machine learning pipelines using Coarsage and PRESTO decision tree algorithms to predict MLB game outcomes and over/under scenarios.

- Evaluated model performance against Vegas odds, achieving 57.2% accuracy and positive returns in simulated betting experiments.
- Analyzed model limitations and sources of uncertainty inherent in sports outcome prediction.
- Highlighted the need for continuous model refinement and adaptive strategies in non-stationary data environments.

Hydrogen Adsorption Energy on Palladium (Pd [111]) November 2023

First-principles surface modeling using density functional theory to study adsorption energetics.

- Investigated hydrogen adsorption energies on Pd (111) surfaces across multiple adsorption sites.
- Performed ab-initio quantum mechanical simulations using the Vienna Ab initio Simulation Package (VASP) with slab supercell models.
- Analyzed adsorption energy variations to identify the most energetically favorable binding configurations.
- Validated computational results through comparison with existing computational and experimental literature.

PUBLICATION

- **Bandyopadhyay, Y.**, Avlani, H., & Zhuang, H. (2025). Kolmogorov–Arnold neural networks for high-entropy alloys design. *Modelling and Simulation in Materials Science and Engineering*, 33(3), 035005.

OTHER EXPERIENCE

Graduate Research Associate Aug 2023 – Present

Interdisciplinary research in machine learning, quantum computing, and materials discovery. *Ira A. Fulton Schools of Engineering, Arizona State University*

Quantum Mechanical Engineering Laboratory

Advisor: Dr. Houlong Zhuang

- Conducting interdisciplinary research at the intersection of classical machine learning, quantum computing, and computational materials science.
- Developing data-driven and physics-informed models for high-entropy alloy (HEA) design and materials screening.
- Applying neural networks, generative AI approaches, and quantum algorithms to accelerate materials discovery workflows.
- Collaborating with academic and industry researchers; contributing to peer-reviewed publications.