Yagnik Bandyopadhyay

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SUMMARY

PhD researcher combining machine learning, generative models, and atomistic simulation for computational materials discovery. Experienced in developing data-driven and physics-informed workflows for property prediction, materials screening, and scientific discovery.

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

EXPERIENCE

Applied Materials – Materials Simulation Engineer Intern May 2026 – Aug 2026
Santa Clara, CA

- Developed GNN-based work-function prediction and materials-informatics workflows to accelerate screening of electrode materials for semiconductor devices; delivered a user-facing inference tool for experimentalists.
- Built MLIP and DFT workflows to evaluate precursor adsorption and surface interactions across oxide materials for semiconductor process applications.

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.

PUBLICATIONS

- **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.
- **Bandyopadhyay, Y.**, Serrao, D. N., & Zhuang, H. L. (2026). Large language model assisted discovery of optimal dopants for enhanced thermoelectric performance in $CoSb_3$-based skutterudites. *arXiv preprint* arXiv:2604.06048.

ACADEMIC PROJECTS

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.

HONORS & AWARDS

- **Make Possible Award**, Applied Materials (2026).

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.

CERTIFICATIONS

Variational Algorithm Design Nov 2024

IBM Quantum Learning

Variational algorithms, ansatz design, cost functions, optimization loops, referenced states.

Machine Learning Specialization Feb 2024

DeepLearning.AI

Supervised learning, advanced algorithms, unsupervised learning, recommenders, reinforcement learning.

Basics of Quantum Information Jan 2024

IBM Quantum Learning

Quantum circuits, entanglement, multi-system formalism.

Fundamentals of Quantum Algorithms Jan 2024

IBM Quantum Learning

Quantum query algorithms, phase estimation, Grover's algorithm.

Introduction to Aerospace Structures and Materials Dec 2018

edX – TU Delft

Structural mechanics, materials selection, fatigue and damage tolerance in aircraft systems.