

Yagnik Bandyopadhyay

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EDUCATION

Doctor of Philosophy, Mechanical Engineering

August 2023-Present

Arizona State University • Tempe, AZ

Relevant Courses: Quantum Mechanics, Applied Linear Algebra, Applied Machine Learning for Mechanical Engineers

Master of Science, Aerospace Engineering

August 2021-May 2023

Arizona State University • Tempe, AZ

Relevant Courses: High Performance Computing, Linear Algebra, Partial Differential Equations, Advanced Numerical Method for PDEs

RESEARCH EXPERIENCE

Visiting Researcher – Generative AI for Electrochemistry

Long Program, Fall 2024

University of California • Los Angeles, CA

- Conducted research at UCLA on generative AI methods (autoregressive and diffusion models) for molecular structure generation in electrochemical systems.
- 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

Hydrogen Adsorption energy on Palladium (Pd [111])

Arizona State University • November 2023

- Investigated hydrogen adsorption energy on Pd surfaces at different adsorption sites.
- Utilized quantum mechanical ab-initio calculations in Vienna Ab initio Simulation Package (VASP) with a Pd [111] supercell.
- Conducted simulations revealing adsorption energy variations across different sites, identified the most stable adsorption site.
- Obtained reasonable adsorption energy results aligned with existing literature (computational and experimental).

Predicting Baseball Game Outcome Using Machine Learning

Arizona State University • November 2023

- Developed and implemented a machine learning model using Coarsage and PRESTO decision tree algorithms to predict Major League Baseball game outcomes and over/under betting scenarios.
- Evaluated model against Vegas odds, demonstrating 57.2% accuracy and a profit of \$3500 in simulated betting.
- Acknowledged challenges in sports prediction and highlighted the need for continuous model refinement.

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.

SKILLS

Programming: Qiskit, Python, Matlab, Fortran

Simulation Package: Vienna Ab-Initio Simulation Package

Frameworks & Libraries: PyTorch, TensorFlow, Scikit-learn, Keras, Qiskit

Data Analysis Libraries: Pandas, NumPy

Design/ Visualization Software: Vesta, Solid Works, Creo, ANSYS, Abaqus

Online Courses/Certifications

Variational Algorithm Design

IBM Quantum Learning • November 2024

- Topics covered – Variational Algorithms, Referenced states, Ansatzes and Variational Forms, Cost functions, Optimizations Loops, Instances and Extensions

Machine Learning Specialization

DeepLearning.AI • February 2024

- Topics covered – Supervised Machine Learning- Regression and Classification, Advanced Learning Algorithms, Unsupervised Learning, Recommenders, Reinforcement Learning

Basics of Quantum Information

IBM Quantum Learning • January 2024

- Topics covered – Single systems, Multiple systems, Quantum Circuits, Entanglement in action

Fundamentals of Quantum Algorithms

IBM Quantum Learning • January 2024

- Topics covered – Quantum Query Algorithms, Quantum algorithmic foundations, Phase estimation and factoring, Grover's algorithm

Introduction to Aerospace Structures and Materials

Edx TU Delft • December 2018

- Learned the basic principles of Structural Mechanics used in the design of Commercial aircraft, and the selection of materials, loads, and stresses acting on the aircraft. Also, I learned about safety, design philosophies, and fatigue and damage tolerances of Commercial aircraft.