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 2025**
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.