

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

Bachelor of Technology, Mechanical Engineering

June 2017-July 2021

Heritage Institute of Technology • Kolkata, India

Relevant Courses: Physics 2(Quantum Physics), Mathematical Methods, Numerical and Statistical Methods

SUMMARY

Passionate about machine learning and materials science, focusing on classical and quantum machine learning algorithms to accelerate the discovery of novel materials. Committed to advancing computational methods for impactful innovations in material design.

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

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

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.