

## SUMMARY OF COMPETENCIES

- Seven years hands-on academic and research experience in data science and machine learning.
- Five years of experience in managing scientific projects and applying statistical data analysis techniques, quantum chemical methods, and high-performance computing to solve research problems and accelerate the discovery of novel materials to combat global challenges in clean energy.
- A tangible record of successful collaborations and completion of independent projects through publications in journals and conference presentations
- Strong programming in Python and experience with Machine learning libraries such as NumPy, Pandas, Scikit-learn, SciPy, PyTorch, and XGBoost.

## EDUCATION

### **Doctor of Philosophy (Ph.D.), Chemical Engineering**

*GPA: 3.98/4.0*

Tulane University, New Orleans, LA

### **Master of Science, Chemical Engineering**

*GPA: 3.98/4.0*

Tulane University, New Orleans, LA

## EXPERIENCE

### **Machine Learning Researcher**

**2018 – Present**

**Department of Chemical Engineering, Tulane University, New Orleans, LA**

- Successfully designed, implemented, and published outcomes of five projects over a four-year period, ensuring efficient use of resources and minimizing rework.
- Responsible for data preprocessing, feature engineering, and analysis of extremely messy scientific data with tools such as SQL, Tableau, Python (Pandas, Numpy, Scikit-learn, Scipy).
- Experience with version control systems such as Git and experience with collaborative coding environments such as GitHub and BitBucket.
- Developed a predictive, interpretable model to understand the factors that control oxophilicity and carbophilicity in pure metal surfaces.
- Developed a general, reusable model to screen alloy surfaces for various catalytic reactions.
- Developed a recommendation system for adaptive experimental design using Bayesian optimization for the discovery of single atom alloys in catalysis.
- Created high standard data visualization outputs using such as Matplotlib, Seaborn, Plotly, Bokeh, Tableau, and Microsoft power-point.
- Gave theoretical guidance to experimentalists by performing quantum-chemical calculations (density functional theory) and structural analysis of catalytic systems.
- Shared research output in peer-reviewed publications, scientific conferences, and open-source software.

### **Scientific Software Developer & Data Scientist**

**Summer 2022**

**Enthought Incorporation, Austin, TX**

- Developed machine learning solutions to tackle polymer formulation scale-up issues for a client R&D company, saving them about \$90,000 per formulation scale-up.
- Created a Bayesian optimization framework to help lab researchers optimize polymer film thickness and also to understand some of the factors that determines this thickness.
- Investigated the use of different surrogate models (like XGBOOST, KRR, SVR) instead of standard Gaussian process regressor (GPR) for Bayesian optimization using the spin coating problem.

### **Senior Data Scientist**

**2022**

**FreeAlas (non-profit organization), New Orleans, LA**

- Collaborated with the Salesforce team to build an efficient ETL pipeline for data automation into Salesforce.
- Utilized analytical expertise to derive insight on donors and fundraising campaign activities using Tableau, Python and Salesforce.

#### **Data Scientist**

**2016 - 2018**

##### **Krosk Partners Limited, *Global consulting***

- Transformed financial data into insights that informed, identified trends, answered questions, and provided recommendations based on project specific goals.
- Researched, analyzed market trends, and collaborated with traders to develop optimal market strategies.
- Contributed to team building, client retention, and business goodwill through prompt delivery of project assigned responsibilities
- Created visualizations and dashboards using Excel and Tableau to communicate insights to stakeholders.

#### **Production Engineer (Intern)**

**2015**

##### **Addax Petroleum, *Global consulting***

- Contributed to the development of predictive models for asset production based on reservoir indicators.
- Gained skills training in Asset integrity and well work executions.
- Performed Asset integrity audits on Pressure safety valves (PSV's) for all the company's producing assets.
- Used SQL, Excel, to monitor daily asset productions and equipment performance.

### **SKILLS**

- Strong programming in Python and experience with machine learning libraries such as NumPy, Pandas, Scikit-learn, SciPy, and PyTorch, XGBoost.
- Excellent analytical, teamwork, and communication skills.
- Proficient with MS Office (Word, Access, Excel, PowerPoint), Tableau, SQL, Git, MATLAB.
- Expertise in machine learning, deep learning, data science and data visualization.
- Adept at quantum-chemical simulations, high-performance computing and computational chemistry.

### **EXTRA-CURRICULAR ACTIVITIES**

- Partnered with the United States Army eCYBERMISSION STEM education initiative as a volunteer judge for science competitions from 2019 to present
- Mentored undergraduates in computational materials research at the Tulane SMART REU program.
- Teamed with undergraduate students at Tulane University as volunteer instructors to support the STEM NOLA education initiative for K-12 students in New Orleans communities.
- Vice president at Tulane's chapter of the National Society of Black Engineers.
- Volunteer at Louisiana FIRST® LEGO® League (FLL) Robotics State Championship.

### **AWARDS**

- 2022 Graduate scholarship, Society for Mining, Metallurgy & Exploration.
- 2022 NSBE Fulfilling Legacy Award, National Society of Black Engineers
- 2022 NSBE BCA/Affiliate/ Fellows Scholarship, National Society of Black Engineers
- 2021 AADE Scholarship Award, American Association of Drilling engineers
- 2021 Anchor Achievement Scholarship Award, Pilot International Inc
- 2021 National Association of Surface Finishing Graduate Award, NASF Foundation
- 2021 NSBE BCA/Affiliate/ Fellows Scholarship, National Society of Black Engineers
- 2020 AKA EAF Graduate Awards, Alpha Kappa Alpha Educational Advancement Foundation
- 2020 AADE Scholarship Award, American Association of Drilling engineers
- 2020 NSBE Apex Scholar, National Society of Black Engineers
- 2020 Anchor Achievement Scholarship Award, Pilot International Inc
- ISA PMCD Scholarship Award, International Society of automation

- Graduate Achiever Scholarship Award, Honor Society
- National Association of Surface Finishing Graduate Award, NASF Foundation
- Rosagene Huggins Memorial Award, ESA Foundation
- Serc Endowment Award, ESA Foundation
- First Class Honors, Covenant University
- Award of Excellence, Covenant University

## ML/PYTHON PROJECTS

- Developed machine learning solutions to predict product delivery dates for an e-commerce company. (**Paid project**). Sample code used for pre-processing [here](#)
- Developed a crypto bot for arbitrage trading between a centralized (Coinbase) and a de-centralized (Kucoin) platform.
- Developed a novel latent variable machine learning framework for predicting adsorption energies of bi-metallic alloys.
- Developed a novel Bayesian optimization framework for discovering Single atom alloys (SAA) for different chemical reactions.
- Developed a simple model to understand oxophilic and carbophilic tendencies in Pure metals.
- Co-developed a novel machine learning framework for screening thousands of alloy catalysts for 7 different reactions.

## OPEN-SOURCE SOFTWARE

- [Surf-ep](#) (Surface energetics predictions for catalysis)
- [Crypto arbitrage bot](#) (Crypto Arbitrage bot)
- [Vibrational modes](#) (Vibrational modes for computational chemistry)

## CONFERENCES

- 2022 Annual AIChE conference. (Poster Presentation)
- 2022 Annual AIChE conference. (Oral Presentation)
- 2021 NOBCCHE Conference. (Oral Presentation)
- 2021 ACS Spring Conference. (Oral Presentation)
- 2020 Annual AIChE conference. (Oral Presentation)

## PUBLICATIONS

- Kayode, G. O., Montemore, M. M. Factors controlling Oxophilicity and Carbophilicity of Transition Metal and Main Group Metals. *J. Mater. Chem. A*. 2021.
- Kayode, G. O., Zhang S., Montemore, M. M. Linking electronic structure to adsorption energies: Metal surfaces and single-atom catalysts. *Catalysis Vol. 34*. Royal Society of Chemistry. 2022
- Montemore, M. M., Nwaokorie, C. F., Kayode, G. O. General screening of Surface Alloys for Catalysis. *Catal. Sci. Technol.* **2020**, *10* (13), 4467–4476.
- Ojewumi, M. E., Kayode, G. O., Omoleye, J., & Oyekunle, D. T. (2019). Statistical optimization and sensitivity analysis of rheological models using cassava starch. *International Journal of Civil Engineering and Technology (IJCIET)*, *10*(1), 623-639
- Kayode, G. O., Montemore, M. M. Latent variable Machine learning framework for catalysis. *In Review*. 2023.
- Wang, J., Kayode, G. O., Hirayama, Y., Ogino, I., Montemore, M. M., Gazit, O. M. Interface between thin MgAlO<sub>x</sub> and ZrO<sub>2</sub> identified as a stabilizing site for highly active Ni catalyst in the DRM. *In Review*. 2023.