# Gbolade "Kay" Kayode

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## 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** **Expected graduation May 2023**
*GPA: 3.98/4.0*
Tulane University, New Orleans, LA

**Master of Science, Chemical Engineering** **May 2022**
*GPA: 3.98/4.0*
Tulane University, New Orleans, LA

**Bachelor of Science, Chemical Engineering** **June 2016**
*First class Honors*
Covenant University, Nigeria

## EXPERIENCE

**Machine Learning Graduate Research Assistant** **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 (PhD intern)** **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 (Ku-coin) 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 $MgAlO_x$ and $ZrO_2$ identified as a stabilizing site for highly active Ni catalyst in the DRM. *In Review*. 2023.