

TESLIM OLAYIWOLA

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HIGHLIGHTS

Process & Data Scientist with extensive experience in **numerical modeling**, **molecular dynamics (MD)**, and **machine learning (ML)** applied to material and process modeling. Skilled in **catalyst synthesis**, **industrial collaborations**, and **leadership roles** within student organizations. Passionate about **positions** that integrate **hybrid modeling**, **MD**, **ML**, and **optimization** techniques, with a strong emphasis on **cross-functional collaboration** to drive innovation in material design and process optimization.

EDUCATION

PhD in Chemical Engineering | Louisiana State University | GPA: 3.92 01/2021 - 12/2024 (expected)

Thesis: Multi-Scale Modeling of Electrochemical Systems: From Property Prediction to Process Optimization

MSc in Petroleum Engineering | African University of Sci. & Tech., Nigeria | GPA: 3.64 06/2016 - 12/2017

BSc in Chemical Engineering | Ladoke Akintola University of Tech., Nigeria | GPA: 3.70 01/2011 - 12/2015

EXPERIENCE

Doctoral Candidate | Louisiana State University, LA 01/2022 - present

Advisor: Professor Jose Romagnoli

- Developed a hybrid modeling framework for electrochemical separation systems, such as electro dialysis and electrodeionization, discovering new optimized conditions with 99% ion separation efficiency & 50% energy savings.
- Devised an ML-based structure-property model for ion activity in membranes, integrating chemical structure, MD simulation, & experiment; improved predictive accuracy by 40%.
- Established 'ImputeNet,' a transfer learning protocol for capacitive deionization modeling, improving predictive accuracy and introducing novel experimental conditions with 300% improvement.
- Proposed novel CuSn_x catalysts and experiments conditions for electrochemical reduction of CO_2 to valuable C_2+ products, utilizing a combination of experiment, ML, and optimization.
- Building robust physics-informed ML models for selective ion separation of biochemical extracts.

Doctoral Research Assistant | Louisiana State University, LA 05/2021 - 12/2021

Advisor: Professor Kunlun Ding (*transferred to Jose Romagnoli's group*)

- Pioneered a surface inorganometallic synthesis protocol to deposit uniform ultra-small (<3nm) Pt-M (M=In, Ga, Cu) supported catalyst; improved adsorption efficiency by 100% and eliminated Pt-Pt bridge.
- Analyzed CO adsorption spectra of Pd nanocrystals, identifying peak reordering post-calcination, enhancing understanding by 30%.

Data Science Intern | Dow Chemical, MI 05/2023 - 08/2023

- Executed end-to-end data collection processes, expertly extracting chemical structures and numerical data from reports, ensuring accurate and error-free data entry into the ML regression pipeline.
- Developed graph-based ML models with >90% accuracy using DGL and PyTorch to surfactant formulation screening, reducing screening time by 30% (if implemented), and deployed with StreamLit.

Research Assistant | Dhahran Techno Valley, Saudi Arabia 01/2019 - 12/2020

- Bolstered HPAM polymer hydrodynamic size by 50% via side chain functionalization for high temperature & high salinity applications using MD simulations, leading to a 30% improvement in performance.
- Conducted DFT simulations, revealing a 20% decrease in water adsorption in kerogen-water systems with maturation, increasing efficiency by 15%.
- Designed ML models for reservoir, ionic liquid and cement properties, achieving with accuracy >98%.

- Boosted Chevron gas flow consistency by 12% using PipeSim, Excel, and JMP, resulting in a 15% reduction in operational downtime & ensuring effective communication with business partners & customers.
- Facilitated a Gas Sales Agreement for a 70mmScf/d supply to Dangote, contributing to a 5% increase in annual revenue.
- Amplified gas supply reliability with daily monitoring protocols, achieving a 20% reduction in supply interruptions.

PROJECTS

- Physics-Informed ML: Developed hybrid model to optimize features in electrochemical systems such as electro-dialysis and electrodeionization.
- Active Learning (AL): Applied different AL sampling techniques and Bayesian Optimization to understand protein adsorption on polymer brushes.
- Failure detection in ESP pumps: Performed Time-series forecasting using statistical & ML methods like LSTM to estimate ESP run life, ranked 3rd in BPX ML Challenge (out of 30 submissions); awarded for code reproducibility.
- Machine Learning Operations (MLOps): Completed data processing and ML deployment pipelines using MLflow, Docker, Mage, AWS, and GIT.

SKILLS

Qualities: Process Modeling, Numerical Modeling, Data Science, Machine Learning, Experimental Design.

AI/ML: PyTorch, Keras, TensorFlow, Scikit-Learn, MLflow, Docker, Terraform, StreamLit, AWS.

Chemistry/Chem Eng: Aspen Plus, GROMACS, LAMMPS, Gaussian, CP2K, DeepChem, RDKit.

Data Engineering: Pandas, Numpy, jupyter-notebook, Excel, JMP.

Languages: Python, MATLAB, GIT, Linux.

Experiment: Catalyst synthesis, Nanocrystals synthesis, Spectroscopy with CO DRIFTS.

PUBLICATIONS

- **T. Olayiwola**, L. Briceno-Mena, C. Arges, R. Kumar, J. Romagnoli, “*Synergizing data-driven and knowledge-based hybrid models for ionic separations*”, Accepted in [ACS ES&T Engineering](#).
- **T. Olayiwola**, R. Kumar, J. Romagnoli, “*Empowering Capacitive Devices Harnessing Transfer Learning for Enhanced Data-Driven Optimization*”, [ACS Ind. Eng. Chem. Res. 2024](#).
- **T. Olayiwola**, K. Gallage Dona, L. Briceno-Mena, C. Arges, R. Kumar, J. Romagnoli, “*Determining ion activity coefficients in ion-exchange membranes with machine learning and molecular dynamics*”, [ACS Ind. Eng. Chem. Res. 2023](#).
- **T. Olayiwola**, S. Abdel-Azeim, “*Insights into atomistic Study of Partially Hydrolyzed Polyacrylamide polymers for Enhanced Oil Recovery application*”, [KFUPM Research report 2020](#).
- O. Lawal, **T. Olayiwola**, S. Abdel-Azeim, M. Mahmoud, A. Onawole, M. Kamal, “*Molecular simulation of kerogen-water interaction Theoretical insights into maturity*”, [Elsevier J. Mol. Liq. 2020](#).

AWARDS

- Winner, BPX Machine Learning Challenge (2024) - 3rd out of 30 submissions.
- Corteva Delta Industry Symposium (2024) - 1 of 15 successful candidates.
- 3M RISE Industry Symposium (2023 & 2024) - 1 of 33 successful candidates.
- Dow BEST Industry Symposium (2023) - 1 of 30 successful candidates.
- Omicron Delta Kappa Society (2022) - out of 1000+ candidates.
- Winner, Society of Petroleum Engineers African Regional Paper Contest (2017) - 1st out of 20+ candidates.
- Best Graduating Chemical Engineering Student (2016) - 1st out of 65 students.
- MTN Foundation Scholarship (2013) - out of 5000 applicants.

LEADERSHIPS AND MENTORING

- Senator, LSU Student Union Government - Enact laws and lobby to improve students' experience.
- Mentor, LSU Genesis Mentoring Program - Advised 1st year undergraduates on college life.
- Vice President, Chemical Eng. Grad. Student Association - Organized workshops and social events.