

TESLIM OLAYIWOLA

Doctoral Candidate | tolayi1@lsu.edu | teslim404.com | Baton Rouge, LA.

HIGHLIGHTS

At Louisiana State University, I developed a unique approach that integrated machine learning, molecular dynamics, and experiments to gain insight into ion activity in ion exchange membranes, which is critical to the design of electrochemical systems. Prior to that, I synthesized and regenerated catalysts using a surface inorganometallic approach for dehydrogenation reactions. I collaborated with Saudi Aramco to create a new polymer using molecular dynamics simulations, and I conducted a DFT simulation study of the impact of maturity on water intake in kerogen. Through these projects, I have acquired proficiency in a range of experimental characterization and computational techniques, which are listed in my skills section (refer to publications).

EDUCATION

Doctor of Philosophy (Ph.D.) in Chemical Engineering	Jan. 2021 – Dec. 2024
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Minor: Computer Science

Louisiana State University, LA, USA.

CGPA of 4.06/ 4.0

Master (M. Sc.) in Petroleum Engineering

Jul. 2016 - Dec 2017

African University of Science and Technology, Abuja Nigeria.

CGPA of 3.64/ 4.0

Bachelor (B.Sc.) in Chemical Engineering

Jan. 2011 - Dec. 2015

Ladoke Akintola University of Technology, Oyo State, Nigeria.

CGPA of 4.62/ 5.0

PROFESSIONAL/WORK EXPERIENCE

Data Science ADISE Intern | Dow Core (FAMS) R&D, US | May 2023 – August 2023

- I successfully developed a graph-based and large language data-driven model to predict the properties of surfactants in aqueous solution, aiding rapid property screening.
- I designed an approach to extend the graph-based method to other pure surfactant properties and mixtures.
- I proposed a graph-based data-driven framework to predict odor and odor threshold of volatile organic compounds in paints.

Doctoral Research Assistant | Cain Department of Chemical Engineering, Louisiana State University Baton Rouge, US | May 2022 – present

- I successfully conducted atomic-scale modeling of the solvation environment in an ion exchange membrane, resulting in improved understanding of ion hydration and dissociation in electrochemical devices.
- I designed a framework that bridges time scales using a data-driven approach, integrating atomic simulations, experiments, and machine learning to build a model that understands the chemistry of constituent molecules present in an electrochemical device.
- I led the development of a multiscale model of electrochemical systems, including electrodeionization and membrane capacitive deionization, using a chemistry-savvy transfer learning approach. This novel framework provides an improved method for assessing the design of membranes and resins for selected electrochemical systems.

Graduate Research Assistant | Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, US | Jan 2021 – May 2022

- I successfully developed a precise approach for depositing ultra-small nanoparticles on catalyst supports via surface inorganometallic synthesis.
- I optimized ligand removal in nanocrystals using UV Ozone and plasma treatment, which allowed for the preservation of the crystal structure without any disruption, unlike conventional techniques like calcination.
- I have successfully analyzed the IR spectra analysis of palladium and platinum nanocrystals using CO DRIFTS, and identified the presence of strong bridging on palladium and reduced CO bridging on platinum, providing valuable insights for further research in this field.

Research Assistant | Dhahran Techno Valley, Dhahran, Saudi Arabia | Jan 2019 – Dec. 2020

- I designed and proposed structural upgrades to HPAM polymer for usage in high temperature and high salinity water with the aid of molecular dynamics tools. Tech: GROMACS, HPC, Python, & Gaussian.
- I developed an approach to study the effect of surfactant charged head group on the interfacial dynamics between water and hydrocarbon. Tech: GROMACS, HPC, Python, & Gaussian.

Graduate Gas Analyst | Chevron Nigeria Limited, Lagos, Nigeria | Aug. 2018 – Dec. 2018

- I led monitoring of Chevron Nigeria gas sales activities and provided routine reports to internal stakeholders, JV partners, and business collaborators parties.
- I designed and optimized workflow for daily gas monitoring and activities at Chevron stations in Escravos.
- I collaborated on the preparation and execution of Gas Sales Aggregation and Agreements for new customers.

SKILL SET

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- **Analysis and Materials characterization:** X-ray diffraction (XRD), Extended X-ray absorption fine structure (EXAFS), X-ray Absorption Near Edge Structure (XANES), Diffuse Reflectance IR Fourier Transform Spectroscopy (DRIFTS), UV etching and Design of Experiment (DoE)
 - **Languages:** Python, SQL, MATLAB
 - **Machine learning:** Scikit-Learn, TensorFlow, Keras
 - **Tools:** GROMACS, LAMMPS, VMD, Gaussian
 - **Platforms:** Linux, Git
 - **Soft Skills:** Research, Leadership, Event Management
 - Proficiency in the use of Microsoft Office Power Point, Word, Excel, and others

AWARDS and HONORS

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- Dow BEST – 2023
 - 3M RISE – 2023
 - NSBE BCA/Affiliate/Fellows Scholarship, National Society of Black Engineers – 2022
 - Omicron Delta Kappa – 2022
 - George Daniel Fellowship – 2021
 - LSU Foundation Graduate Assistantship – 2021

SELECTED PEER-REVIEWED PUBLICATIONS

- **Olayiwola T**, Briceno-Mena L, Arges C, Kumar R, Romagnoli J. A Hybrid Modeling Framework for Electrochemical Separation Systems: Combining Compositional Modeling and Machine Learning. *Manuscript in preparation*
- **Olayiwola T**, Nnadiokwe C, Dauda M, Arges C, Kumar R, Romagnoli J. Computational Modeling of Electrochemical Separation Processes with Machine Learning and Molecular Dynamics: A review — Manuscript submitted to *ACS Environ. Sci. Technol.*
- **Olayiwola T**, Gallage Dona K., Briceno-Mena L, Arges C, Kumar R, Romagnoli J. Determining ion activity coefficients in ion-exchange membranes with machine learning and molecular dynamics. *Ind. Eng. Chem. Res.* 2023, 62, 24, 9533–9548
Google scholar page: <https://scholar.google.com/citations?user=ao5QIMgAAAAJ&hl=en>

CONFERENCES/SYMPOSIUM ATTENDED

- 2023 AIChE Annual Meeting (11/05/2023 – 11/10/2023).
Poster presentation: Automated Synthesis of Hybrid Models for Ionic Separations
- 2023 NOBCCChE Conference (09/11/2023 – 09/14/2023).
Poster presentation: Integrating Physics and Machine Learning: A Hybrid Modeling Approach for Electrochemical Separation
- 2022 ACS Southwest Regional Meeting conference (11/06/2022 – 11/09/2022).
Poster Presentations: Understanding bimetallic formation via aided inorganometallic complexation.

LEADERSHIP POSITIONS HELD

- Vice President, Chemical Engineering Graduate Student Association, LSU. May. 2022 – May 2023.
- Vice President, African Graduate Student Association, LSU. May. 2022 – May 2023.
- Member-at-Large, International Student Association, LSU. Sept. 2022 – May 2023.
- Membership Chair, African Graduate Student Association, LSU. May. 2021 – June 2022.

MENTORING

2022 Fall Genesis Mentoring Program at LSU

08/2022 – 12/2022

I mentored underrepresented Americans admitted to Louisiana State University on how to navigate their first year of university study.

2021 Fall Research Mentoring Program at LSU

09/2022 – 12/2022

I mentored two high school kids for a Summer Research training on synthesis and characterization of catalyst.

PROFESSIONAL AFFILIATIONS

- American Institute of Chemical Engineers (AIChE) – Student Member.
- American Chemical Society (ACS) – Student Member
- National Society of Black Engineers (NSBE) – Collegiate Member.
- National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCCChE) – Student Member.