

TESLIM OLAYIWOLA

Doctoral Candidate | NIW EB2 recipient | tolayi1@lsu.edu | teslim404.com | Baton Rouge, LA.

HIGHLIGHTS

Versatile PhD candidate proficient in multiscale modeling of electrochemical separation, atomic-scale modeling of macromolecules (polymers, surfactants), and small molecules (solvent, electrolytes), as well as adept in machine learning modeling of materials; with hands-on experience in catalyst synthesis and collaboration with industries, showcasing leadership and mentorship skills.

EDUCATION

Doctor of Philosophy (Ph.D.) in Chemical Engineering <i>Minor: Computer Science / Advisors: Prof. Jose Romagnoli</i> Louisiana State University (LSU), LA, USA.	Jan. 2021 – Dec. 2024 (expected) GPA: 4.0/ 4.0
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Master (M. Sc.) in Petroleum Engineering African University of Science and Technology, Abuja Nigeria.	Jul. 2016 – Dec 2017 GPA: 3.64/ 4.0
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Bachelor (B.Sc.) in Chemical Engineering Ladoke Akintola University of Technology, Oyo State, Nigeria.	Jan. 2011 – Dec. 2015 GPA: 4.62/ 5.0
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Honors/Awards: NOBCChE Conference Grant awardee (2022, 2023); Dow BEST awardee (2023); 3M RISE awardee (2023); Omicron Delta Kappa (2022); George Daniel Fellowship 2021; Winner, Society of Petroleum Engineers' African Paper Contest (2017); MTN Foundation Scholar (2013)

PROFESSIONAL/WORK EXPERIENCE

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

- Developed a graph-based and large language data-driven model to predict surfactant properties in aqueous solutions, expediting the screening process for formulation.
- Designed an approach extending the graph-based method, resulting in significant improvement in predicting pure surfactant properties and mixtures.

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

Advisors: Professor Jose Romagnoli & Revati Kumar

- Conducted atomic-scale modeling of the solvation environment in membranes, resulting in improved understanding of ion hydration and dissociation in electrochemical devices.
- 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 molecules present in an electrochemical device.
- Led the development of a multiscale model of electrochemical systems, including electrodialysis, electrodeionization and capacitive deionization, using a chemistry-savvy transfer learning approach.
- Collaborated on the use of Generative models and Molecular simulations in developing new surfactant molecules with desired molecular property.

Doctorial Research Assistant | Cain Department of Chemical Engineering, LSU, Baton Rouge, US | Jan 2021 – May 2022

Advisor: Professor Kunlun Ding

- Developed a precise approach for depositing ultra-small nanoparticles on catalyst supports via surface inorganometallic synthesis.

- Analyzed the IR spectra analysis of nanocrystals using CO DRIFTS, and identified the presence of strong bridging on palladium and reduced CO bridging on platinum.

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

Advisor: Dr Safwat Abdelazeim

- Designed and proposed structural upgrades to HPAM polymer for usage in high temperature and high salinity water with the aid of molecular dynamics tools.
- Developed an approach to study the effect of surfactant charged head group on the interfacial dynamics between water and hydrocarbon.

Graduate Intern | Chevron, Lagos, Nigeria | Aug 2018 – Dec. 2018

- Collaborated on design and optimization of daily gas monitoring workflows at Chevron stations in Escravos, ensuring seamless operations.
- Provided routine reports on gas facilities operations to internal stakeholders, joint venture partners, and business collaborators.
- Played a key role in the Gas Sales Aggregation and Agreement processes for Dangote Fertilizer, Sahara Energy, and Olorunsogo Power Plant, demonstrating expertise in managing complex negotiations and collaborations within the energy sector.

SKILL SET

- **Machine learning & Optimization:** Scikit-Learn, PyTorch, TensorFlow, Pymoo, BoTorch
- **Tools:** GROMACS, LAMMPS, Gaussian, Aspen Plus
- **Languages:** Python, MATLAB
- **Office:** Power Point, Word, Excel

SELECTED PEER-REVIEWED PUBLICATIONS

- M. Nnadili M., Okafor A. N, **Olayiwola T**, Akinpelu D, Romagnoli J. A Generative AI-Driven Molecular Design: Combining Predictive Models and Reinforcement Learning for Tailored Molecule Generation. *Preprint published in ChemRxiv*
- **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**, 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>

SELECTED LEADERSHIP & MENTORING EXPERIENCE

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| • Vice President, Chemical Eng. Graduate Student Association. | May. 2022 – May 2023 |
| • Vice President, African Graduate Student Association. | May. 2022 – May 2023 |
| • Member-at-Large, International Student Association. | Sep. 2022 – May 2023 |
| • Membership Chair, African Graduate Student Association. | May. 2021 – June 2022 |
| • Mentor, LSU Genesis Mentoring Program | Aug. 2022 – Dec. 2022 |
| • Mentor, LSU Research Mentoring Program | Sep. 2022 – Dec. 2022 |