MOHAMMED AL OTMI

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RELEVANT PROFESSIONAL EXPERIENCES

Energy Frontier Research Center (Remote)

Computation & Informatics Researcher *Dec. 2022 – May.2025*

- Led two projects on anion exchange membrane fuel cells (AEMFC) within the $36M DOE-funded Energy Frontier Research Center (EFRC), managed goals and timelines, and presented the results at 4 conferences.
- Integrated molecular dynamics with machine learning to screen 11 million copolymer candidates for anion exchange membrane materials, identifying top performers with >120 mS/cm conductivity and <35% water uptake.
- Investigated the impact of ion-ion correlation using Onsager framework and devised innovative approach to estimate the contribution of Grotthuss transport (proton hopping) using classical molecular dynamics simulations.
- Collaborated with experimental teams to design fluorine-rich poly(arylene amine) membranes, reducing energy costs and carbon emissions for hydrocarbon separations by 2-10 times based on technoeconomic analysis.

University of Florida (Gainesville, Florida)

Graduate Research Assistant *Aug. 2020 – May.2025*

- Developed a high-throughput framework that uses Molecular Dynamics and Monte Carlo to examine free volume architecture in polymer membranes, boosting performance and durability through rational, data-informed design.
- First to illustrate the correlation between local segmental dynamics and free volume stability in polymer membranes, and determine their impact on penetrant diffusion.
- Established a quantitative structure-property relationship (QSPR) model to predict polymer density and glass transition temperature using a curated dataset of ~ 13,000 homopolymers.
- Developed a theory-informed regression model to predict polymer adsorption properties using data curated from molecular simulations, achieving 85% confidence level.

Delta Protein International (Sunflower, Mississippi)

Product Quality Engineer *May. 2020–Aug. 2020*

- Performed daily chemical and microbial tests to ensure product quality including PH, viscosity, high-performance liquid chromatography (HPLC), conductivity, color and clarity, and standard plate count (SPC).
- Conducted weekly effluent tests to ensure safe water discharge with contaminants below 5% of compliance limits.
- Developed a standard operating procedure to ensure testing efficiency and maintain product quality, including troubleshooting steps to identify and resolve process issues impacting chemical or microbial compliance.
- Performed scale-up calculations to size new ion exchange columns that use a cheaper and more efficient resin.

Mississippi State University (Starkville, Mississippi)

Undergraduate Researcher *Aug. 2018 –May. 2019*

- Synthesized polystyrene N,N di-carboxymethyl dithiocarbamate (PSDC) in polymer solution, characterized its structure using Fourier Transform Infrared Spectroscopy (FT-IR), and examined its stability as a function of crosslinking.
- Prepared high-concentration heavy metal solutions, including lead, copper, and nickel, to evaluate resin performance.
- Assessed resin capacity by measuring the change in concentrations using Atomic Absorption Spectroscopy (AAS).
- Achieved a 20% ion removal and presented outcomes at the 2019 Mississippi Water Resource Conference.

EDUCATION

University of Florida (Gainesville FL)

Ph.D. in Chemical Engineering (GPA: 3.97/4.0) *Aug. 2020 – May.2025*

- Awards: 2024 CHE Research Excellence Award, UF GSC Travel Award, Elias Klein Founder's Award from North American Membrane Society Conference, AIChE Excellence in Graduate Polymer Research Award.
- Mentoring: Trained new students, developed manuals, Teaching Assistant for Separation and Mass Transfer Operations.
- Workshops: Machine Learning for Molecular Science Summer School (i-CoMSE), Laboratory Scale Reactor Design (Dow Chemical), Data-driven Materials Innovation (Schrodinger), Supervised Machine Learning (DeepLearningAI).

MSc. in Chemical Engineering (GPA – 3.97/4.0) *Aug. 2020 – May 2024*

Mississippi State University (Starkville MS)

BSc. in Chemical Engineering (GPA – 3.73/4.0) *Aug.2016 – May. 2019*

- *Minor in Political Science and Public Administration*, Undergraduate Researcher, Dean Scholar.
- Awards: Winner of 2018 Undergraduate Research Stipend, Phi Theta Kappa Scholarship, Maron & White Scholarship, Top-10 Scholarship for Undergraduate Studies (Ranked 7th of 218,964 students in Yemen National High School Exams).

SKILLS AND INTERESTS

- **Technical Skills:** Design of Experiments (DOE), CHEMCAD, Aspen Plus, Technoeconomic Analysis, Process Flow Diagrams (PFDs) and Piping and Instrumentation Diagrams (P&IDs).
- **Laboratory Techniques:** Atomic Absorption Spectroscopy (AAS), High-Performance Liquid Chromatography (HPLC), Fourier Transform Infrared Spectroscopy (FT-IR).
- **Computational Skills**: Python (data analysis, simulation automation), Bash, High Performance Computing, Machine Learning (Scikit-learn, Pytorch), Computational Chemistry (Molecular Dynamics Simulations, DFT), MATLAB.
- **Molecular Simulation Packages:** LAMMPS, GROMACS, GAUSSIAN.
- **Non-technical Skills:** Cross-functional Collaboration, Project Management, Public Speaking, Leadership.
- **Personal Interests:** Hiking, Photography, Tennis, Languages (Bilingual: Arabic & English, Currently Learning Spanish).

SELECTED PUBLICATIONS

- Al Otmi, M.; Colina, C.; Lively, R.; Sampath, J. "Free Volume Elements in Polymer Membranes: Theory, Characterization, Functional Significance, and Design Strategy" *Book Chapter in Computational Methods for the Multiscale Modelling of Soft Matter, edited by Paola Carbone and Nigel Clarke,* ***Elsevier Inc*** *(Under Review).*
- Schertzer, W.; Shukla, S.; Al Otmi, M.; …; Sampath, J.; Lively, R; Ramprasad, R. "AI-Driven Design of Fluorine-Free Polymers for Sustainable and High-Performance Anion Exchange Membranes" ***Journal of Material Informatics*** *(2025).*
- Yi, R.; Hui, M.; Kim, J.; Al Otmi, M.; ..., Sampath, J.; Realff, M.; Lively, R.; Guo, S. "Fluorine-Rich Poly(Arylene Amine) Membranes for the Separation of Liquid Aliphatic Compounds" ***Science*** *(2025).*
- Al Otmi, M.; Lin, P.; Schertzer, W.; Colina, C.; Ramprasad, R.; Sampath, J. "Investigating Correlations in Hydroxide Ion Transport in Anion Exchange Membranes from Atomistic MD Simulations" ***ACS Applied Polymer Materials*** *(2024).*
- Al Otmi, M.*; Wernisch, B.*; Sampath, J. "Evolution of free volume elements in amorphous polymers undergoing uniaxial deformation: a molecular dynamics simulations study" ***Molecular Systems Design & Engineering*** *(2024,* *equal contribution)
- Al Otmi, M.; Willmore, F.; Sampath, J. "Structure, Dynamics, and Hydrogen Transport in Amorphous Polymers: An Analysis of the Interplay between Free Volume Element Distribution and Local Segmental Dynamics from Molecular Dynamics Simulations" ***Macromolecules*** *(2023).*

CONFERENCES AND PROFESSIONAL TALKS

American Institute of Chemical Engineers (AIChE) Annual Meeting

- "Probing Polymer Relaxation and Plasticization Dynamics Using MD Simulations" Oral Presentation (2024, San Diego CA).
- "Exploring the Contributions of Vehicular and Grotthuss Diffusion Mechanisms in Anion Exchange Membranes" Poster Presentation (2024, San Diego CA).
- "Investigating Ion Transport, Mechanical Properties, and Stability of Tetraalkylammonium-Functionalized Polyethylene" Oral Presentation (2023, Orlando FL).
- "Effect of Chain Dynamics on the Free Volume Elements of Glassy Polymers from Atomistic Molecular Dynamics Simulations" Oral Presentation (2022, Phoenix AZ).

Foundations of Molecular Modeling and Simulation Conference

- "Navigating Polymer Membrane Design: Balancing Durability and Performance" Poster Presentation (2024, Snowbird UT).

North American Membrane Society Conference

- "Modeling Permeation in Polymer Membranes Using Non-Equilibrium Molecular Dynamics Simulations" Oral Presentation (2023, Tuscaloosa AL).

National Organization for the Professional Advancement of Black Chemists and Chemical Engineers

- "Unraveling Membrane Mysteries: Molecular Insights for Polymer Design in Gas Separation and Ion Exchange Applications" Oral Presentation (2024, Orlando FL).

UF GRACE Symposium

- "Modeling Permeation in Polymer Membranes using Non-Equilibrium MD Simulations" Poster (2023, Gainesville FL).
- Atomistic Modelling of Hydrogen Diffusion in Polystyrene, Polymethylpentene, and HAB-6FDA Thermally Rearranged Polymers" Oral Presentation (2022, Gainesville FL).

33rd IUPAP Conference on Computational Physics

- "The Dynamic Nature of Free Volume Element and its Effect on the Performance of Glassy Polymers Using Atomistic Molecular Dynamics Simulations" Oral Presentation (2022, Austin TX).

Mississippi Water Resource Conference

- "Experimental Study of the Performance of the N, N'- di (carboxymethyl) dithicarbamate Chelating Resin in Removing Heavy Metals from Oilfield Wastewater" Poster Presentation (2019, Jackson MS).