Mohammed Al Otmi

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SUMMARY

Ph.D. Chemical Engineer with interdisciplinary expertise in polymer science, separation processes, and computational materials design. Skilled in developing simulation tools, applying machine learning, and integrating computational and experimental workflows to accelerate material discovery and product innovation. Proven record of leading cross-functional R&D from molecular science to pilot-scale implementation, with a focus on addressing challenges of translating lab-scale innovations into reliable, industrial-scale solutions.

EDUCATION

Ph.D. & M.S. in Chemical Engineering (GPA:3.97/4.00)   Aug 2020 – May 2025

University of Florida   Gainesville, FL

- Thesis: Understanding Transport Mechanisms in Polymer Membranes Through Molecular Simulations

- Advisor: Dr. Janani Sampath

- 5 publications, 2 manuscripts in preparation, 1 book chapter, 14 conference presentations

B.S. in Chemical Engineering (GPA:3.73/4.00)   Aug 2016 – May 2019

Mississippi State University   Starkville, MS

- Minor in Political Science and Public Administration, Dean's Undergraduate Scholar, AIChE SAChE Safety Certificate

RESEARCH EXPERIENCE

Computation & Informatics Researcher   Dec 2022 – Present

Energy Frontier Research Center (EFRC)   Remote

- Led in-silico screening of fluorine-rich polymer membranes, guiding synthesis teams to develop novel chemistries with 10× higher efficiency for hydrocarbon separation.

- Leveraged machine learning and molecular simulations to screen 11 million anion exchange membrane (AEM) copolymers, identifying 400+ fluorine-free candidates with enhanced conductivity and minimal water uptake.

- Developed an efficient framework to capture ion–ion correlations and proton hopping physics in AEM candidates, improving conductivity calculations without costly first principle simulations.

Graduate Research Assistant   Aug 2020 – May 2025

University of Florida   Gainesville, FL

- Built a high-throughput framework that uses molecular dynamics and Monte Carlo to predict and analyze free volume element(FVE) in polymer membranes, accelerating materials screening and design.

- Applied customized MD/MC workflow to screen poly(glycolic acid) (PGA)-based materials with controlled free volume architecture and tailored adsorption properties, supporting a $1.5M NSF–industry collaboration to design sustainable, high-barrier packaging materials with improved processability and degradability.

- Built a theory-informed model predicting polymer gas adsorption with 85% accuracy, integrating machine learning screening with molecular simulation validation

Undergraduate Researcher   Aug 2018 – May 2019

Mississippi State University   Starkville, MS

- Synthesized dithiocarbamate-functionalized resin for removing heavy metals from oilfield produced water.

- Conducted batch adsorption studies with Cu, Pb, and Ni and achieved ∼20% removal within 10 minutes.

- Quantified resin adsorption capacity by measuring concentration changes via atomic absorption spectroscopy (AAS).

INDUSTRY EXPERIENCE

Pilot-scale Consultant   May 2025 – July 2025

Renovo Resources LLC   Bakersfield, CA

- Supported the design and led night operations of a pilot-scale Ultra-High Pressure Reverse Osmosis (UHPRO) system for treating produced water at 1,800 psi.

- Directed the night-shift pretreatment operations to control hardness and minimize membrane scaling via chemical softening and WAC resin polishing, enabling UHPRO treatment of produced water up to 120,000 ppm TDS.

- Coordinated and performed engineering, operational, and testing activities to monitor membrane integrity and verify water quality, ensuring reliable UHPRO system performance.

- Maintained safety compliance, logged operational data, and documented results to inform scale-up and deployment.

Product Quality Engineering Intern   May 2020 – Aug 2020

Delta Protein International   Sunflower, MS

- Performed weekly effluent testing on treated water, ensuring contaminant levels (COD, TSS, DO, ammonia, chlorine) remained below 5% of regulatory discharge limits.

- Conducted daily product quality tests: pH, viscosity, conductivity, moisture, standard plate count (SPC), etc.

- Developed a standard operating procedure (SOP) to ensure testing efficiency and maintain product quality.

LEADERSHIP & MENTORSHIP

- **AEM project leader, EFRC**: Coordinated goals, timelines, and meetings; presented updates at EFRC meetings.

- **Lab manager, Sampath Research Group**: Trained 6 students; created lab manuals and video tutorials.

- **Participant, NSF MFS-SPEED initiative**: Collaborated with chemists and data scientists in an NSF–industry program (BASF, Dow, IBM, P&G, PepsiCo) to advance sustainable polymer discovery and manufacturing through AI/ML and data-driven research.

- **Teaching assistant for Separation & Mass Transfer Operations**: Held office hours; delivered lectures; graded exams.

- **Treasurer and sport chair, Graduate Association of Chemical Engineers, University of Florida:** Organized sporting events; managed budget and allocated funds for events; participated in recruitment and peer-mentoring program.

- **Co-founder and vice president, Yemeni Student Association, Mississippi State University:** Co-founded the first Yemeni student group on campus; grew membership to 14+; organized a cultural showcase at the International Fiesta with 1,500+ attendees.

RELEVANT SKILLS

- **Programming & Data Science:** Python, Bash, Git, Machine Learning (Regression/Classification, Molecular Fingerprinting, Neural Networks – PyTorch, Scikit-Learn).

- **Computational & Simulation Tools:** Molecular Dynamics (LAMMPS, GROMACS), Monte Carlo, Ab Initio/DFT (Gaussian), High-Performance Computing.

- **Process Engineering:** Scale-up, Pilot-scale Testing, Process Troubleshooting, CHEMCAD, Technoeconomic Analysis.

- **Experimental Techniques:** Analytical Testing (HPLC, AAS, FT-IR), Post-polymerization Functionalization, Water Quality Analysis.

- **Management & Communication:** Cross-functional Collaboration, Project Leadership, Mentorship, Grant Writing, Stakeholder Engagement, Scientific Communication.

- **Languages:** English (Professional Proficiency), Arabic (Professional Proficiency).

SELECTED AWARDS

- **UF:** AIChE Excellence Award in Graduate Polymer Research (2024), UF Research Excellence Fellowship (2024), Elias Klein Founder's Award from North American Membrane Society (2023)

- **MSU:** Undergraduate Research Stipend (2018), Non-Resident Scholarship (2016-2019), Phi Theta Kappa Scholarship (2016-2018), Maroon White Scholarship (2017)

SELECTED PUBLICATIONS

- Al Otmi, M., Colina, C., Lively, R., Sampath, J. "Free Volume Elements in Polymer Membranes" ***Book Chapter in Computational Methods for the Multiscale Modelling of Soft Matter***, **Elsevier Inc**, *In Press*.

- Schertzer, W., Shukla, S., Rafiq, R., Al Otmi, M., . . . , Ramprasad, R. "AI-Driven Design of Fluorine-Free Polymers for Sustainable and High-Performance Anion Exchange Membranes" ***Journal of Materials 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., Willmore, F., Sampath, J. "Structure, Dynamics, and Hydrogen Transport in Amorphous Polymers" ***Macromolecules***, 2023.

- Al Otmi, M.*, Wernisch, B.*, Sampath, J. "Evolution of Free Volume Elements in Amorphous Polymers Undergoing Uniaxial Deformation" ***Molecular Systems Design & Engineering***, 2024. (*equal contribution)

- Al Otmi, M., Lin, P., Schertzer, W., Gissenger, J., Ramprasad, R., Sampath, J. "Grotthuss Contribution in Anion Exchange Membranes: Insight from Classical Molecular Dynamics Simulations" *In Preparation*

- Schertzer, W., Al Otmi, M., Sampath, J., Lively, R., Ramprasad, R. "Uncovering Universal Degradation Behavior of Anion Exchange Membranes with Physics-Enforced Neural Networks" *In Preparation*

SELECTED PRESENTATIONS

- **American Institute of Chemical Engineers (AIChE) Annual Meeting:** *"Probing Polymer Relaxation and Plasticization Dynamics Using Molecular Dynamics Simulations"*. Oral Presentation, 2024, San Diego, CA.

- **American Institute of Chemical Engineers (AIChE) Annual Meeting:** *"Exploring the Contributions of Vehicular and Grotthuss Diffusion Mechanisms in AEMs"*. Poster, 2024, San Diego, CA.

- **Foundations of Molecular Modeling and Simulation (FOMMS):** *"Navigating Polymer Membrane Design: Balancing Durability and Performance"*. Poster, 2024, Snowbird, UT.

- **National Org. of Black Chemists Chemical Engineers (NOBCChE):** *"Unraveling Membrane Mysteries: Molecular Insights for Polymer Design in Gas Separation and Ion Exchange Applications"*. Oral Presentation, 2024, Orlando, FL.

- **North American Membrane Society (NAMS):** *"Modeling Permeation in Polymer Membranes Using Non-Equilibrium Molecular Dynamics Simulations"*. Oral Presentation, 2023, Tuscaloosa, AL.

- **American Institute of Chemical Engineers (AIChE) Annual Meeting:** *"Investigating Ion Transport, Mechanical Properties, and Stability of Tetraalkylammonium-Functionalized Polyethylene"*. Oral Presentation, 2023, Orlando, FL.

- **33rd IUPAP Conference on Computational Physics (CCP):** *"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.

- **American Institute of Chemical Engineers (AIChE) Annual Meeting:** *"Effect of Chain Dynamics on the Free Volume Elements in Glassy Polymers"*. Oral Presentation, 2022, Phoenix, AZ.

- **Mississippi Water Resource Conference (MWRC):** *"Experimental Study of the Performance of the N,N'-di(carboxymethyl) dithicarbamate Chelating Resin in Removing Heavy Metals from Oilfield Wastewater"*. Poster, 2019, Jackson, MS.