Mohammed Al Otmi

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SUMMARY

Ph.D. chemical engineer with expertise in polymer science and computational materials design. Skilled in leveraging structure–property relationships through data-driven screening, molecular simulations, and experimental validation. Passionate about renewable energy and sustainable separation technologies.

EDUCATION

University of Florida Gainesville, FL

Ph.D. & M.S. in Chemical Engineering, GPA: 3.97 Aug 2020 – May 2025

- Thesis: Understanding Transport Mechanisms in Polymer Membranes Through Molecular Simulations
- Workshops: ML for Molecular Science (i-CoMSE), Lab-scale Reactor Design (Dow), Data-driven Material Innovation (Schrodinger), Supervised Machine Learning (DeepLearningAI)

Mississippi State University Starkville, MS

B.S. in Chemical Engineering, GPA: 3.73 Aug 2016 – May 2019

- Minor in Political Science, AIChE Safety & Chemical Engineering (SAChE) Certificate, Dean's Undergraduate Scholar

PROFESSIONAL EXPERIENCE

Energy Frontier Research Center (EFRC) Remote

Computation & Informatics Researcher Dec 2022 – Present

- Led DOE-funded projects on anion exchange membranes (AEM), managing timelines and presenting at 4 conferences.
- Collaborated within a multidisciplinary team to design fluorine-rich poly(arylene amine) membranes with up to 10x energy/cost savings for hydrocarbon separations.
- Used MD + ML to screen 11M copolymers, revealing transport physics of top candidates.
- Devised a model capturing ion correlation and proton hopping in AEMs, improving simulation-experiment agreement.

University of Florida Gainesville, FL

Graduate Research Assistant Aug 2020 – May 2025

- Built a high-throughput MD/MC framework for analyzing free volume in polymer membranes.
- Illustrated the correlation between chain dynamics to free volume element stability and penetrant diffusion.
- Developed a QSPR ML models predicting density and T_g from 13k+ homopolymers.

Delta Protein International Sunflower, MS

Product Quality Engineering Intern May 2020 – Aug 2020

- Used HPLC to characterize collagen hydrolysates, ensuring controlled enzymatic breakdown into low molecular weight peptides (less than 5 kDa) for enhanced solubility and bioavailability.
- Conducted daily quality tests: pH, viscosity, conductivity, moisture, color and clarity, standard plate count (SPC), etc.
- Created GMP-compliant SOP and implemented AVEVA Historian for real-time quality tracking.

Mississippi State University Starkville, MS

Undergraduate Researcher Aug 2018 – May 2019

- Synthesized dithiocarbamate-modified resin for removing heavy metals from water and verified structure via FTIR.
- 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).

TECHNICAL SKILLS

- **Programming & Scripting:** Python, Bash, High-Performance Computing (HPC)
- **Machine Learning & Modeling:** Scikit-learn, Bayesian Optimization, QSPR Models
- **Computational Chemistry:** Molecular Dynamics (LAMMPS, GROMACS), Monte Carlo, DFT (Gaussian)
- **Experimental & Analytical Tools:** HPLC, AAS, FT-IR, DOE, Post-polymerization Functionalization
- **Process Engineering:** Scale-up, Equipment Sizing, PFDs, P&IDs, Troubleshooting, Technoeconomic analysis
- **Software & Platforms:** AVEVA Historian, Git, LaTeX, Microsoft Office Suite, CHEMCAD
- **Languages:** English (Professional Proficiency), Arabic (Professional Proficiency)

LEADERSHIP & MENTORSHIP

- Led AEM projects at EFRC; coordinated goals, teams, and reporting.
- Trained 6+ students; created lab manuals and software tutorials.
- Teaching assistant and guest lecturer for Separations and Mass Transfer Operations class.
- Treasurer and sport chair for Graduate Association of Chemical Engineers (GRACE); peer mentor for incoming students.
- Co-founded the Yemeni Student Association at MSU; helped in organizing a cultural showcase with 1,500+ attendees.

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), Phi Theta Kappa Scholarship (2017), Non-Resident Scholarship (2016)
- **High School:** The Top-Ten Student scholarship for Undergraduate Studies from the Yemeni government (2013)

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.*, 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., Willmore, F., Sampath, J. "Structure, Dynamics, and Hydrogen Transport in Amorphous Polymers" ***Macromolecules***, 2023.
- Al Otmi, M., Lin, P., Gissenger, J., Sampath, J. "Exploring the Grotthuss Mechanism in Hydroxide Transport Using the REACTER Framework" *In Preparation*.

CONFERENCES & 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.
  - *"Exploring the Contributions of Vehicular and Grotthuss Diffusion Mechanisms in AEMs"*. Poster, 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 in Glassy Polymers"*. Oral Presentation, 2022, Phoenix, AZ.
- **Energy Frontier Research Center (EFRC) All-hands Meeting:**
  - *"Capturing Grotthuss Diffusion in Anion Exchange Membranes"*. Poster, 2025, Atlanta, GA.
  - *"Simulations for Insight into AEM Performance and ML-Generated Candidates"*. Poster, 2024, Atlanta, GA.
- **Foundations of Molecular Modeling and Simulation (FOMMS):** *"Navigating Polymer Membrane Design: Balancing Durability and Performance"*. Poster, 2024, Snowbird, UT.
- **National Organization for the Professional Advancement of Black Chemists and 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.
- **UF GRACE Symposium:** *"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 (CCP):** *"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 (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.

REFERENCES

Dr. Janani Sampath (PI)
Assistant Professor, University of Florida
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Dr. Jason Gorski
General Manager, Delta Protein International
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