

Highlights

- Expert in catalysis, environmental engineering and electrochemistry.
- Computational expertise in mathematical and multiscale molecular modeling.
- Experimental expertise in electrochemical and data characterization techniques.
- Solid teaching and mentoring experience.
- 20 years of industrial experience.
- Extensive computer knowledge:
 - Macroscale Software: MATLAB, Maple, and Aspen Plus.
 - Microscale software: Gaussian, VASP, and Lammmps.
 - Programming: Python, Fortran.

Education

- PhD in Chemical Engineering** **May 2018**
Ohio University, Athens, OH, **GPA 3.90/4.00**
Dissertation Title: "Mathematical and molecular modeling of ammonia electrolysis with experimental validation"
- Master of Science in Chemical Engineering** **Jul. 1999**
Shiraz University, Iran.
- Bachelor of Science in Chemical Engineering** **Dec. 1996**
Shiraz University, Iran.

Research, Teaching, and Industrial Experience

Tennessee Technological University, Chemical Engineering Department **Cookeville, TN**
<https://www.tntech.edu/engineering/programs/che/index.php> **Sep 2024- Present**
Assistant Professor

Lafayette College, Department of Chemical and Biomolecular Engineering **Easton, PA**
<https://che.lafayette.edu/> **Jul. 2022-Aug 2024**
Visiting Assistant Professor

- Instructor for "Engineering Thermodynamics", "Transport Phenomena", "Material and Energy Balances", "Applied Fluid Mechanics and Heat Transfer"

Clemson University, Department of Chemical and Biomolecular Engineering, **Clemson, SC**
www.clemson.edu/cecas/departments/chbe/ **Aug. 2019 – Sep. 2022**
Postdoctoral Research Associate

- Multiscale molecular modeling of solvent and external electric field on electrocatalyst surface. The influence of the "double layer" on electrocatalytic phenomena is an outstanding knowledge gap that has plagued the catalysis community for over 40 years. We used multiscale modeling to elucidate the thermodynamic and kinetics of chemical (particularly methanol oxidation) reaction on the interface.

Ducon Environmental Technologies INC., **Farmingdale, NY**
www.duconenv.com/ **Aug. 2019 – Present**
Sr. Technical Consultant

Ducon Environmental Technologies INC., **Farmingdale, NY**
www.duconenv.com/ **Apr. 2016 – July 2019**

Sr. Technical Engineer

- Project engineering and management with complex scope of works. This includes basic design, PFD and PID preparation, reactor vessels, pumps, and piping system, fan and ducting system design (work as a team member and in some cases as team leader).
- Project leader:

Project Description	Unit(s)	Customer	Value
Chlorine and Hydrochloric Acid Separation	Quencher, Packed Tower	Durr, USA	\$770,000
Particulate and SO ₂ Removal	Multi Cyclones, Multi Rods	CEMTEC, Austria	\$1,000,000

- Writing proposal for environmental and chemical units like absorption, adsorption, packed towers, scrubbers, Flue Gas Desulfurization (FGD) units in oil and gas industry, and Fluidized Catalytic Cracking (FCC) units.

Ohio University, Athens, OH, USA, www.ohio.edu/engineering/chemical 2011-Apr. 2016
 Graduate research and teaching assistant at center for electrochemical engineering research (CEER)

- Mentored two (2) undergraduate students and serving as TA for “Introduction to Chemical Engineering”.
- Developed kinetics of ammonia electrolyzer for hydrogen production as a clean energy and wastewater remediation technology. I expanded a model which predicts the ammonia removal from wastewater:
 - Established a comprehensive Fortran code considering transport phenomena and kinetics of heterogeneous catalyst.
 - Manufactured a parallel plate bench scale ammonia electrolyzer prototype to validate the model, including platinum electrodeposited on nickel mesh substrate working as anode electrode, RDE experiments to determine HER (hydrogen evolution reaction) kinetics for nickel mesh cathode.
 - Analyzed the results to examine limiting factors in performance as well as identified areas of deficiency in the model and redefined some parts of the model to enhance it.
- Theoretical investigation (Density Functional Theory) of ammonia oxidation to determine an efficient catalyst:
 - Examined the reaction mechanism on platinum and iridium monometallic clusters. Found the deactivation mechanism of the electrode and promoting suggestion to utilize platinum-iridium bimetallic surface.
 - Performed thermochemical evaluations of the reaction mechanism through frequency analysis to determine kinetics parameters.
 - Compared the parameters with experimental results of literature.
- Electrodeposition of platinum and iridium on nickel to reduce the quantity of noble metals and developed an economic and enhanced catalyst for ammonia oxidation process in a scale up system.

Azad University, Iran (<http://www.miau.ac.ir/>) 2010-2011

Instructor

- Instructor for “Unit Operation” course in chemical engineering.

ShayanTarh Co, Iran, www.shayantarh.com 2007- 2011

Basic and sales engineering manager, project manager

GrIn Co, Iran, www.griinco.com 1998-2007

Basic and sales engineering manager, project manager

- Wrote technical and financial proposal for more than 500 projects and secured more than \$50,000,000.

- Performed technical audit for variety of de-dusting equipment in different industries (cement, steel, power plants) worldwide.
- Performed R&D on de-dusting equipment.

Service

- Session chair for SECS, South-Eastern Catalysis Society symposium, 2020
- Vice president of ECS student chapter at Ohio University (2012-2015).
- ECS student chapter representative in ElectrochemOhio conference at the Ohio State University (2014).
- Strategic planning and management.

Publications and Presentations

Publications

- **A. Estejab**; R. B. Getman, Water/Solid Interface in Thermal- and Electrocatalysis for Wetting and Non-Wetting Surfaces: Interactions and Models. In *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*; Elsevier, 2023.
- R. A. Garcia Carcamo, X. Zhang, **A. Estejab**, J. Zhou, B. J. Hare, C. Sievers, S. Sarupria, R. B. Getman, , “Differences in solvation thermodynamics of oxygenates at Pt/Al₂O₃ perimeter versus Pt(111) terrace sites,” *iScience*, vol. 26, no. 2, p. 105980, Feb. 2023,.
- **A. Estejab**, R. A. García Cárcamo, and R. B. Getman, “Influence of an electrified interface on the entropy and energy of solvation of methanol oxidation intermediates on platinum(111) under explicit solvation,” *Phys. Chem. Chem. Phys.*, vol. 24, no. 7, pp. 4251–4261, 2022.
- **A. Estejab**, and G.G. Botte, “Ammonia oxidation kinetics on bimetallic clusters of platinum and iridium: a theoretical approach,” *J. of Molecular Catalysis A: Chemical*, 445, pp. 279-292, 2018.
- **A. Estejab**, and G.G. Botte, “DFT calculations of ammonia oxidation reactions on bimetallic clusters of platinum and iridium,” *J. of Computational and Theoretical Chemistry*. 1091, p31, 2016.
- **A. Estejab**, D. A. Daramola, and G. G. Botte, "Mathematical model of a parallel plate ammonia electrolyzer for combined wastewater remediation and hydrogen production," *Water Research*, vol. 77, pp. 133-145, 2015.
- **A. Estejab** and B. Khorrami Saadi, "ESP for Iranian upgrade," *World Cement*, vol. 37, pp. 35-36, 2006
- **A. Estejab**, “Solving thermodynamic unbalances problem of Gas Conditioning Tower” Sep. 1999 Iranian cement magazine, A translation from an article in world cement, Jan. 1999 by Rischter O., Taylor R

Presentations (14, most recents)

- Ali Estejab, Ricardo A. García Cárcamo, Rachel B. Getman, “Electrified Interface influence on the Entropy and Energy of Solvation of Methanol Oxidation Intermediates on Platinum(111) Under Explicit Solvation.” Oral presentation at **NAM27 New York, May 2022**.
- Ali Estejab, Rachel B. Getman, “Influence of an external potential on the solvation thermodynamics of intermediates in the pathway for methanol oxidation on Pt(111)”, Oral presentation at **AIChE Boston, November 2021**.
- Ali Estejab, Rachel B. Getman, “Effect of potential and explicit aqueous media on oxidation process on Pt(111) using computational multi-scale modeling”, Oral presentation at **SECS virtual symposium September 2020** and **AIChE virtual meeting November 2020**.
- Ali Estejab, Gerardine G. Botte, “Theoretical calculations of ammonia oxidation kinetics on platinum, iridium and their bimetallic clusters. Oral presentation at **ECS Conference, San Diego, May-June. 2016**

- Ali Estejab, Gerardine G. Botte, “Optimized performance of a scale-up ammonia electrolyzer”, Oral presentation at **ECS Conference, Chicago, May. 2015**
- Ali Estejab, Luis A. Diaz, Gerardine G. Botte, “De-ammonification of wastewater through ammonia electrolysis”, Oral presentation at **ECS Conference, San Francisco Oct-Nov 2013**

Honors and Awards

- **Student Travel Grant**
Electrochemical society, 2015.
- **Chapter of Excellence**
Vice president of Ohio University electrochemical society student chapter, 2013-14.
- **Ohio University's Research and Creative Activity Expo**
2nd prize, 2012.
- **Company of Excellence**
Department manager at GrIIIn Inc. with 50 percent of country market share for de-dusting equipment.
- **Top Ten Finisher**
Hydrogen student design contest, 2012.
- **Student of Excellence**
2nd among 70 graduates in class of 1995.