MEHDI ZARE, Ph.D.

Research Assistant Professor | Department of Chemical Engineering

University of South Carolina

301 Main Street, Columbia, SC 29208 | mzare@email.sc.edu

Research Interests: Computational catalysis • Molecular simulation • Machine learning • Multiscale modeling • Heterogeneous catalysis

ACADEMIC & RESEARCH APPOINTMENTS

Research Assistant Professor, University of South Carolina (Columbia, SC, USA) (Sep.2026-present)

- Conduct computational research in heterogeneous catalysis, molecular simulation, and machine learning to understand catalytic reactions and accelerate catalyst discovery for sustainable chemical processes.
- Develop multiscale computational frameworks integrating density functional theory (DFT), molecular dynamics (MD), QM/MM, and machine learning potentials to investigate catalytic reactions at solid–liquid and polymer–catalyst interfaces.
- Lead and contribute to collaborative research projects funded by federal agencies and industrial partners in catalysis, plastics upcycling, and carbon management.
- Collaborate with experimental and computational researchers to elucidate reaction mechanisms, interpret experimental observations, and guide catalyst design through predictive modeling.
- Mentor graduate and undergraduate researchers in computational catalysis, molecular simulation, scientific writing, and research project development.
- Develop competitive research proposals and contribute to securing external funding from DOE, NSF, and other federal and industrial sponsors.

Associate Scientist, University of South Carolina (Columbia, SC, USA) (Sep.2024-Sep.2026)

- Advisor: Andreas Heyden, PhD
- Contributed to writing multiple proposals submitted to DOE and NSF.
- Studied aqueous-phase effects in hydrogen adsorption over transitions metals.
- Investigated the reaction mechanism of 2-butanone hydrogenation to 2-butanol in water over Ru-based catalysts explaining the root cause of increased activity observed experimentally.
- Mentored and counseled graduate students in different projects.

Postdoctoral Researcher, University of South Carolina (Columbia, SC, USA) (Sep.2023-Sep.2024)

- Advisor: Andreas Heyden, PhD
- Developed a hybrid QM/MM scheme to investigate the polymer melt phase effects on energetics of reactions involved in catalytic upcycling of plastic waste at polymer-catalyst interface.
- Mentored and counseled graduate students in different projects.

Postdoctoral Researcher, University of Delaware (Newark, DE, USA) (Aug.2021-Aug.2023)

- Advisor: Dionisios G. Vlachos, PhD
- Developed a scheme to investigate interfacial polymer-catalyst interactions using simulations and data science towards developing next-gen catalysts for chemical recovery of plastics.
- Guided experimentalists how plastic additives or different added solvents to the feedstock can impact reaction yields of plastics upcycling process.
- Collaborated with experimentalists to design novel catalysts and processes for recycling/upcycling of plastic wastes.
- Mentored and counseled graduate students in different projects.

Graduate Research Assistant, University of South Carolina (Columbia, SC, USA) (Aug.2016-Aug.2021)

- Awarded outstanding graduate student research award.
- Contributed to a $550,000 research grant funded by DOE developing an innovative approach to investigate adsorption processes in liquid.
- Developed a multiscale QM/MM model (*eSMS*) for catalysis at solid-liquid interfaces.
- Developed a machine learning (ML) model using Python to quantify the solvent effect in heterogenous catalysis for *in-silico* catalyst discovery.
- Developed a neural network (NN) force field to describe the catalyst-solvent interactions.
- Performed first-principles microkinetic modeling of hydrodeoxygenation of various biomass molecules over transition metal catalysts in vapor and aqueous phases to identify the factors governing the reaction kinetics and thermodynamics.

EDUCATION

PhD in Chemical Engineering, University of South Carolina (Columbia, SC, USA) (Aug.2021)
Dissertation: "Solvent effect modeling in heterogenous catalysis" | **Advisor:** Andreas Heyden, Ph.D.

Master of Science in Chemical Engineering, University of Tehran (Tehran, Iran) (Sep.2013)

Bachelor of Science in Chemical Engineering, Shiraz University (Shiraz, Iran) (Sep.2011)

TEACHING EXPERIENCES

Instructor, University of South Carolina (Columbia, SC, USA) (Spring 2024-present)

- SCHC 370 (HNRS: Science and Design of Coffee)
- ENCP 111 (The Science and Design of Coffee)

Teaching Assistant, University of South Carolina (Columbia, SC, USA) (Fall 2017)

- ECHE 430 (Chemical Engineering Kinetics), ECHE 460, 461 (Chemical Engineering Laboratory)

Undergraduate Student, Shiraz University (Shiraz, Iran) (Sep. 2009- Sep. 2011)

- Organized several group studies and taught and help my classmates to understand and solve engineering problems in courses such as Thermodynamics, Mass Transfer, and Unit Operations

INDUSTRY EXPERIENCES

Design Engineer, PIDEC ***(Petrochemical Industries Design & Engineering Company)*** (Shiraz, Iran) (Feb-Aug 2016)

- Studied and analyzed different projects' PFDs, BFDs, P&IDs, plot plans, etc.

Engineering Intern, Fars Combined Cycle Power Plant (Shiraz, Iran) (June-Sep 2011)

- Maintained and monitored power plant cycles and important units to detect anomaly during its normal operating hours.
- Received hands on training on industrial equipment.

SELECTED PUBLICATIONS

Zare, M.; Watthaisong, P.; Komen, P.; Sahsah, D.; Zeeshan, M.; Heyden, A. *Hydrogen Adsorption over Transition Metals in Water: The Interplay between Solvation and Surface Coverage.* **J. Phys. Chem. C 2026**, *130*, 179–189.

Zare, M.; Sahsah, D.; Saleheen, M.; Behler, J.; Heyden, A. *Atomistic Insights into Aqueous-Phase Carbonyl Hydrogenation over Ru Catalysts from a Hybrid Quantum Mechanical/Molecular Mechanical/Machine Learning Potential.* **ACS Catal. 2026**, *16*, 8702–8718.

Zare, M.; Sahsah, D.; Bamidele, O. H.; Heyden, A. *Polyolefin Melt-Phase Effects on Alkane Hydrogenolysis over Pt Catalysts.* **Chem Catalysis 2024**, *4*, 101093.

Zare, M.; Sahsah, D.; Saleheen, M.; Behler, J.; Heyden, A. *Hybrid Quantum Mechanical, Molecular Mechanical, and Machine Learning Potential for Computing Aqueous-Phase Adsorption Free Energies on Metal Surfaces.* **J. Chem. Theory Comput. 2024**, *20*, 8247–8260.

Zare, M.; Kots, P. A.; Hinton, Z. R.; Epps, T. H.; Korley, L. T. J.; Caratzoulas, S.; Vlachos, D. G. *Effect of Reaction Media on Hydrogenolysis of Polyethylene Plastic Waste: Polymer–Surface Interactions in Small Alkane/Polymer Blends.* **Appl. Catal. B Environ. Energy 2024**, *351*, 123969.

Zare, M.; Kots, P. A.; Caratzoulas, S.; Vlachos, D. G. *Conformations of Polyolefins on Platinum Catalysts Control Product Distribution in Plastics Recycling.* **Chem. Sci. 2023**, *14*, 1966–1977.

Zare, M.; Saleheen, M.; Singh, N.; Uline, M. J.; Faheem, M.; Heyden, A. *Liquid-Phase Effects on Adsorption Processes in Heterogeneous Catalysis.* **JACS Au 2022**, *2*, 2119–2134.

Zare, M.; Saleheen, M.; Kundu, S.; Heyden, A. *Dependency of Solvation Effects on Metal Identity in Surface Reactions.* **Commun. Chem. 2020**, *3*, 187.

Zare, M.; Solomon, R. V.; Yang, W.; Yonge, A.; Heyden, A. *Theoretical Investigation of Solvent Effects on the Hydrodeoxygenation of Propionic Acid over a Ni(111) Catalyst Model.* **J. Phys. Chem. C 2020**, *124*, 16488–16500.