SHUWEN YUE

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EDUCATION / TRAINING

Massachusetts Institute of Technology, Cambridge, MA — Oct. 2021 – Present
Postdoctoral Associate, Department of Chemical Engineering

Princeton University, Princeton, NJ — 2016 – 2021
Ph.D. in Chemical and Biological Engineering
Certificate in Computational Science and Engineering

The University of Alabama, Tuscaloosa, AL — 2012 – 2016
B.S. in Chemical Engineering and Chemistry
Minor in Mathematics and Computer-based Honors

RESEARCH EXPERIENCE

Postdoctoral Associate, Massachusetts Institute of Technology, Cambridge, MA — Oct. 2021 – Present
Advisor: Heather J. Kulik

- Studying molecular transport mechanisms of water and electrolytes in confined nano-materials, as part of the DOE Center for Enhanced Nanofluidic Transport (CENT)
- Applying high-throughput screening and machine learning techniques towards the design of MOFs for biomimetic membranes

Graduate Student Researcher, Princeton University, Princeton, NJ — 2016 – 2021
Advisor: Athanassios Z. Panagiotopoulos

- Elucidated the role of polarizability on water hydration structure from analysis of dynamic and thermodynamic properties of aqueous electrolyte solutions
- Assessed the treatment of long-range physics in atomistic machine-learning models in water and aqueous electrolyte solutions, as part of the DOE Center for Chemistry in Solutions and at Interfaces (CSI)
- Probed specific ion effects in bulk and interfacial aqueous electrolyte solutions properties using atomistic machine-learning models and enhanced sampling techniques
- Assessed vapor-liquid phase behavior of CO_2 using advanced many-body, polarizable models

Undergraduate Student Researcher, The University of Alabama, Tuscaloosa, AL — 2012 – 2016
Advisor: David A. Dixon

- Studied conformation changes of aromatic phosphine ligand complexes using DFT calculations
- Calculated acidities and basicities of biomass derivatives

Advisor: Jason E. Bara

- Designed experimental procedure for the synthesis of tri- and tetra-substituted imidazolium-based ionic liquid monomers for polymer membranes used in separation processes

Advisor: Martin A. Bakker

- Synthesized porous carbon supports for Pd/C catalysts used in hydrogenation reactions

AWARDS AND HONORS

Princeton nominee for the Schmidt Science Fellowship — 2021
WIC Travel Award, The American Institute of Chemical Engineers — 2020
WCC Merck Award, The American Chemical Society [about] — 2020
Best Talk in Computational Modeling, Princeton CBE Graduate Student Symposium [about] — 2019
Mary and Randall Hack '69 Graduate Award, Princeton University [about] — 2019
Andlinger Center for Energy and the Environment Travel Grant, Princeton University — 2019
William R. Schowalter Travel Grant, Princeton University — 2018, 2019
School of Engineering and Applied Science Travel Grant, Princeton University — 2018
Francis Robbins Upton Fellowship, Princeton University — 2016 – 2021
Tau Beta Pi Fellowship [about] — 2016
Tau Beta Pi Scholarship [about] — 2015

Catherine J. Randall Premier Award, The University of Alabama [about] 2016
Alexander Stanton Undergraduate Research Award, The University of Alabama ChBE 2016
Outstanding Chemistry Undergraduate Research Award, The University of Alabama 2016
2016, 2015, 2014 Randall Outstanding Undergraduate Research Award, The University of Alabama [about] 2014 – 2016
2nd Place in 2016, 2nd Place in 2015, 4th place in 2014, Undergraduate Research and Creative Activity Conference, Natural Sciences Division, The University of Alabama 2014 – 2016
1st place, Southeastern Undergraduate Research Conference, Physical and Analytical Chemistry Division 2015

JOURNAL PUBLICATIONS

1. **Yue, S.**, Riera, M.*, Ghosh, R.*, Panagiotopoulos, A. Z., and Paesani, F. Transferability of data-driven, many-body models for CO_2 simulations in the vapor and liquid phases. *Journal of Chemical Physics.* **2022.** 156, 104530. [link]
2. Zhang, C., **Yue, S.**, Panagiotopoulos, A. Z., Klein, M. L., and Wu, X. Dissolving salt is not equivalent to applying a pressure on water. *Nature Communications.* **2022.** 13, 822. [link]
3. Muniz, M. C.*, Gartner III, T. E.*, Knight, C., Riera, M., **Yue, S.**, Paesani, F., and Panagiotopoulos, A. Z. Vapor-liquid equilibria of water using the MB-pol many-body potential. *Journal of Chemical Physics.* **2021.** 154, 211103. Selected as *Featured Article* and *SciLight*. [link]
4. **Yue, S.***, Muniz, M. C.*, Andrade, M. F. C., Zhang, L., Car, R., Panagiotopoulos, A. Z. When do short-range atomistic machine-learning models fall short? *Journal of Chemical Physics.* **2021.** 154, 034111. Selected as *Featured Article.* [link]
5. Kussainova, D., Mondal, A., Young, J. M., **Yue, S.**, Panagiotopoulos, A. Z. Molecular simulation of liquid-vapor coexistence for NaCl: Full-charge vs scaled-charge interaction models. *Journal of Chemical Physics.* **2020.** 153, 024501. [link]
6. **Yue, S.**, Panagiotopoulos, A. Z. Dynamic Properties of Aqueous Electrolyte Solutions from Nonpolarisable, Polarisable, and Scaled-Charge Models. *Molecular Physics.* **2019.** 117 (23-24), pp 3538-3549. [link]
7. Whitley, J. W., Horne, J. W., Andrews, M. A., Terrill, K. L., Hayward, S. S., **Yue, S.**, Mittenthal, M. S., O'Harra, K. E., Shannon, M. S., Bara, J. E. Systematic Investigation of the Photopolymerization of Imidazolium-Based Ionic Liquid Styrene and Vinyl Monomers. *Journal of Polymer Science Part A: Polymer Chemistry.* **2018.** 56, 2364-2375. [link]
8. **Yue, S.**, Roveda, J. D., Mittenthal, M. S., Shannon, M. S., Bara, J. E. Experimental Densities and Calculated Fractional Free Volumes of Ionic Liquids with Tri- and Tetra-substituted Imidazolium Cations. *Journal of Chemical and Engineering Data.* **2018.** 63 (7), 2522-2532. [link]
9. Fang, Z., Both, J., Li, S., **Yue, S.**, Aprà, E., Keçeli, M., Wagner, A. F., Dixon, D. A. Benchmark Calculations of Energetic Properties of Groups 4 and 6 Transition Metal Oxide Nanoclusters Including Comparison to DFT. *Journal of Chemical Theory and Computation.* **2016.** 12, 3689-3710. [link]

* denotes equal contribution

SELECTED PRESENTATIONS

1. **Yue, S.**, Panagiotopoulos, A. Z. Specific ion effects in aqueous electrolyte solutions from first principles derived machine-learning potentials. (*talk*) AIChE Annual Meeting, November 2021.
2. **Yue, S.**, Muniz, M. C., Andrade, M. F. C., Zhang, L., Car, R., Panagiotopoulos, A. Z. Handling long-range interactions in machine-learning models of water and electrolyte solutions. (*talk*) AIChE Annual Meeting, November 2020. [YouTube video]
3. **Yue, S.**, Muniz, M. C., Andrade, M. F. C., Zhang, L., Car, R., Panagiotopoulos, A. Z. Designing machine-learning models of water and aqueous electrolyte solutions. (*invited talk*) Women ExceLling in COmputational Molecular Engineering (WELCOME) Seminar, November 2020.

4. **Yue, S.**, Muniz, M. C., Andrade, M. F. C., Zhang, L., Car, R., Panagiotopoulos, A. Z. Designing machine-learning models of water and aqueous electrolyte solutions. (*talk*) Princeton CBE Graduate Student Symposium. October 2019. (*awarded Best Talk in Computational Modeling session*)
5. **Yue, S.** and Panagiotopoulos, A. Z. Influence of Polarizability on Specific Ion Effects in Aqueous Electrolyte Solution Dynamics. (*Invited talk*) Gordon Research Seminar: Chemistry and Physics of Liquids. July 2019.

PROPOSAL WRITING EXPERIENCE

1. **Co-PI**, NSF XSEDE, "Developing Accurate Materials Design Strategies Across Method- and Length-Scales." PI: Heather J. Kulik. (2022)
2. **Contributor**, DOE INCITE Summit LCF, "Multi-scale, ab initio dynamical simulations of heterogeneous electrochemical aqueous interfaces." PI: Roberto Car. (2021)
3. **Contributor**, DOE BES-CSGB NERSC, "Computational Chemical Science Center: Chemistry in Solution and at Interfaces" PI: Roberto Car. (2020)

TEACHING AND MENTORING EXPERIENCE

Maria Muniz – CBE PhD student, Princeton University 2019 – 2021
Reha Mathur – CBE undergraduate, Princeton University Summer 2021
Andre Guest – CBE Senior Thesis student, Princeton University Fall 2020
Dina Kussainova – Undergraduate summer researcher, Princeton University Summer 2019
(currently PhD student at Princeton CBE)
Ayanna Matthews – Physics Junior Thesis student, Princeton University Spring 2019
(currently PhD student at UChicago Biophysics)
Teaching Assistant, CBE 442 Design, Synthesis, and Optimization of Chemical Processes, Princeton University 2017, 2018
Instructor, University Honors Seminar on Professional Development, The University of Alabama Fall 2015

ACADEMIC AND PROFESSIONAL ACTIVITIES

Student Research Council for DOE CENT EFRC 2022 – Present
Organized weekly seminars and coordinated center-wide communications

Co-Chair, 2023 Gordon Research Seminar: Chemistry and Physics of Liquids 2019 – Present
Secured conference funding from various agencies and journals in collaboration with GRC chairs, organized session topics, and selected speakers and panelists (postponed from 2021 due to COVID-19) [website]

Session Co-Host, Molecular Simulations with Machine Learning Workshop July 2020
Co-hosted hands-on tutorial workshop for using Deep Potential Molecular Dynamics

Journal Reviewer: *Science Advances*
Conference Session Chair:
AIChE 2022: Innovations in Methods of Data Science
ACS Fall 2019: Computational Studies of Water

Professional Memberships: AIChE, ACS

SERVICE AND OUTREACH ACTIVITIES

Secretary/Treasurer, Princeton Graduate Women in Science and Engineering (GWiSE) 2018 – 2020
Developed programs to advocate for inclusion and gender equality in STEM fields at Princeton

President, Princeton Graduate Engineering Council 2017 – 2019
Led a 10-member leadership council which served as the liaison between the graduate student body and School of Engineering and Applied Science (SEAS) administration, organized SEAS-wide professional development and social events, managed budget of $15,000/year

Co-lead, Princeton CBE Recruitment Weekend 2017, 2018
Organized activities and communications for prospective CBE graduate students

Mentor, NYC Girls Computer Science and Engineering Conference November 2018
Mentored 9th and 10th grade girls in NYC high schools to improve their computer science skills and provide career advising [about]

President, U. Alabama Student Chapter of the American Chemical Society 2014 – 2016
Led organization to be named the 2015 Most Outstanding Academic Organization at The University of Alabama, 2015 Honorable Mention for ACS Student Chapter Award by the national ACS Student Chapter Board

Founder and Director, Greener Tide Project 2015 – 2016
Initiated a volunteer based campus-wide recycling initiative to optimize waste management during football tailgating weekends (200,000+ population increase in city limits) in collaboration with University of Alabama Recycling, ESPN College GameDay, and campus partners. Awarded $5000 grant from the Daniel Foundation of Alabama and support of ∼30 student and staff volunteers to carry out project [press]

Team leader, Startup Gauntlet Customer Discovery Boot Camp 2013 – 2014
Led a team of undergraduate students to assess potential markets to apply heterogeneous catalysts produced by the start-up company ThruPore Technologies, Inc. in small-scale biodiesel production, awarded 1st Place at the 2014 University of Alabama Student Prototype Competition

Co-founder and Co-director, STEM Career Exploration Initiative Summer 2013
Co-led an extensive 3-week service project to teach math and physics concepts to a 12th grade Engineering Applications class at Francis Marion High School in Marion, AL to instill interest in STEM related fields and provide career advising. Awarded $800 grant from the University of Alabama Honors College to carry out project