





SHUWEN YUE

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EDUCATION / TRAINING

Massachusetts Institute Technology , Cambridge, MA <i>Postdoctoral Research Associate</i> , Department of Chemical Engineering	2021 – Present
Princeton University , Princeton, NJ <i>Ph.D. in Chemical and Biological Engineering</i> Certificate in Computational Science and Engineering	2016 – 2021
The University of Alabama , Tuscaloosa, AL <i>B.S. in Chemical Engineering and Chemistry</i> Minor in Mathematics and Computer-based Honors	2012 – 2016

RESEARCH EXPERIENCE

Graduate Student Researcher, Princeton University , Princeton, NJ <i>Advisor: Athanassios Z. Panagiotopoulos</i> <ul style="list-style-type: none">– 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– 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 CO₂ using advanced many-body, polarizable models	2016 – 2021
Undergraduate Student Researcher, The University of Alabama , Tuscaloosa, AL <i>Advisor: David A. Dixon</i> <ul style="list-style-type: none">– Modeled conformational changes of aromatic phosphine ligand complexes– Calculated acidities and basicities of biomass derivatives <i>Advisor: Jason E. Bara</i> <ul style="list-style-type: none">– Designed experimental procedure for the synthesis of tri- and tetra-substituted imidazolium-based ionic liquid monomers for polymer membranes used in separation processes <i>Advisor: Martin A. Bakker</i> <ul style="list-style-type: none">– Synthesized porous carbon supports for Pd/C catalysts used in hydrogenation reactions	2012 – 2016

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	2020
Best Talk in Computational Modeling , Princeton CBE Graduate Student Symposium	2019
Mary and Randall Hack '69 Graduate Award , Princeton University	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	2016
Tau Beta Pi Scholarship	2015
Catherine J. Randall Premier Award , The University of Alabama	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	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

PUBLICATIONS SUBMITTED / IN PREPARATION

1. **Yue, S.** and Panagiotopoulos, A. Z. Role of long-range interactions in atomistic machine-learning models of aqueous electrolyte solutions. *In preparation*.
2. **Yue, S.**, Riera, M.*, Ghosh, R.*, Panagiotopoulos, A. Z., and Paesani, F. Thermodynamic properties of CO₂ from many-body polarizable models. *In preparation*.
3. **Yue, S.**, Zhang, C., Wu, X., and Panagiotopoulos, A. Z. Specific ion effects in aqueous electrolyte solutions from ab initio deep neural network models. *In preparation*.
4. Zhang, C., **Yue, S.**, Panagiotopoulos, A. Z., Klein, M. L., and Wu, X. Water-structure modifications in sodium chloride solutions are confined to ionic first solvation shells. *In review*.

JOURNAL PUBLICATIONS

1. 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](#))
2. **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](#)).
3. 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](#)).
4. **Yue, S.**, Panagiotopoulos, A. Z. Dynamic Properties of Aqueous Electrolyte Solutions from Nonpolarisable, Polarizable, and Scaled-Charge Models. *Molecular Physics*. **2019**. 117 (23-24), pp 3538-3549. ([link](#)).
5. 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](#)).
6. **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](#)).
7. 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.**, 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](#))
2. **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.
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. (*talk*) Princeton CBE Graduate Student Symposium. October 2019. (*awarded Best Talk in Computational Modeling session*)
4. **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.
5. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*Invited talk*) The University of Alabama Department of Chemical Engineering Seminar. March 2019.

PROPOSAL WRITING EXPERIENCE

1. **Contributor**, DOE INCITE “Multi-scale, ab initio dynamical simulations of heterogeneous electrochemical aqueous interfaces” on Summit LCF.

TEACHING AND MENTORING EXPERIENCE

Maria Muniz – CBE PhD student , Princeton University	2019 – 2021
Reha Mathur – CBE undergraduate , Princeton University	2021
Andre Guest – CBE Senior Thesis student , Princeton University	Fall 2020
Dina Kussainova – Undergraduate summer researcher , Princeton University (currently PhD student at Princeton CBE)	Summer 2019
Ayanna Matthews – Physics Junior Thesis student , Princeton University (currently PhD student at UChicago Biophysics)	Spring 2019
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

SERVICE AND LEADERSHIP

Co-Chair, 2023 Gordon Research Seminar: Chemistry and Physics of Liquids 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)	2019 – Present
HPC Administrator, Panagiotopoulos group cluster Performed maintenance and monthly updates for 600-core CPU and GPU cluster	2018 – Present
Session co-host, Molecular Simulations with Machine Learning Workshop Co-hosted hands-on tutorial workshop for using Deep Potential Molecular Dynamics as part of the Princeton Chemistry in Solutions and at Interfaces (CSI) center	July 2020
Secretary/Treasurer, Princeton Graduate Women in Science and Engineering (GWISE) Developed programs to advocate for inclusion and gender equality in STEM fields at Princeton	2018 – 2020
President, Princeton Graduate Engineering Council 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	2017 – 2019
Co-lead, Princeton CBE Recruitment Weekend Organized activities and communications for prospective CBE graduate students	2017, 2018
President, U. Alabama Student Chapter of the American Chemical Society 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	2014 – 2016
Session Chair: ACS National Meeting Fall 2019: Computational Studies of Water	
Member: AIChE, ACS	

SKILLS

Computational methods: Molecular Dynamics, Monte Carlo
Programming Language: Python, Bash, C++
Software Tools: LAMMPS, GROMACS, Cassandra (Monte Carlo package), PLUMED, Quantum ESPRESSO, MATLAB, Mathematica