# SHUWEN YUE

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# EDUCATION / TRAINING

Massachusetts Institute of Technology, Cambridge, MA Postdoctoral Research Associate, Department of Chemical Engineering Advisor: Heather J. Kulik	2021 - 2023
<b>Princeton University</b> , Princeton, NJ Ph.D. in Chemical and Biological Engineering Certificate in Computational Science and Engineering Advisor: Athanassios Z. Panagiotopoulos	2016 - 2021
<b>The University of Alabama</b> , Tuscaloosa, AL B.S. in Chemical Engineering and Chemistry Minor in Mathematics and Computer-based Honors Advisors: David A. Dixon, Jason E. Bara, Martin A. Bakker	2012 - 2016

## ACADEMIC APPOINTMENTS

Cornell University, Ithaca, NY July 2023 – Present Assistant Professor, Robert F. Smith School of Chemical and Biomolecular Engineering Affiliate Faculty, Cornell AI for Science Institute

### AWARDS AND HONORS

	202.1
Scialog Fellow, Sustainable Minerals, Metals, and Materials (SM3)	2024
Best Poster Award, Foundations of Molecular Modeling and Simulation (FOMMS)	2022
Early Career Research Award Travel Grant, FOMMS	2022
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	2019
Andlinger Center for Energy and the Environment Travel Grant, Princeton	2019
William R. Schowalter Travel Grant, Princeton	2018, 2019
School of Engineering and Applied Science Travel Grant, Princeton	2018
Francis Robbins Upton Fellowship, Princeton	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	2016
Outstanding Chemistry Undergraduate Research Award, The University of Alabam	a 2016
2016, 2015, 2014 Randall Outstanding Undergraduate Research Award,	2014 - 2016
The University of Alabama	
2nd Place in 2016, 2nd Place in 2015, 4th place in 2014, Natural Sciences,	2014 - 2016
Division, The University of Alabama Undergraduate Research and Creative Activity	
Conference	
1st place, Physical and Analytical Chemistry Division, Southeastern Undergraduate	2015
Research Conference	_010
Dr. Charles L. Seebeck Endowed Scholarship, The University of Alabama	2015
Computer-Based Honors Program Outstanding Sophomore Award,	2013
The University of Alabama	2014
1st Place, Alabama Institute for Manufacturing Excellence Student Prototype	2014
Competition, The University of Alabama	2014

#### PUBLICATIONS

 Yue, S., Nandy, A., and Kulik, H. J. Discovering Molecular Coordination Environment Trends for Selective Ion Binding to Molecular Complexes Using Machine Learning. *The Journal of Physical Chemistry B.* 2023. 127, 49, 10592–10600. [link]

- JPC-B Machine Learning Virtual Special Issue

 Zhang, C., Yue, S., Panagiotopoulos, A. Z., Klein, M. L., and Wu, X. Why dissolving salt in water decreases its dielectric permittivity. *Physical Review Letters.* 2023. 2304893. [link]

- Featured in Science Magazine News

- Roh, H., Yue, S., Hu. H., Chen, K., Kulik, H. J., Gumyusenge, A. Leveraging Polymer Electrochromism for Organic Electrochemical Synaptic Devices. *Advanced Functional Materials*. 2023. 2304893. [link]
- Mathur, R., Muniz, M. C., Yue, S., Car, R., and Panagiotopoulos, A. Z. First-principles-based Machine Learning Models for Phase Behavior and Transport Properties of CO<sub>2</sub>. *The Journal of Physical Chemistry B.* 2023. 127, 20, 4562–4569. [link]
- Nandy, A., Yue, S., Oh, C., Duan, C., Terrones, G. G., Chung, Y. G., and Kulik, H. J. A database of ultrastable MOFs reassembled from stable fragments with machine learning models. *Matter.* 2023. 6, 5, 1585-1603. [link]

- Featured in <u>MIT News</u>

 Yue, S., Oh, C., Nandy, A., Terrones, G. G., and Kulik, H. J. Effect of MOF linker rotation and functionalization on methane uptake and diffusion. *Molecular Systems Design & Engineering.* 2023. 8, 527-537. [link]

- Selected as MSDE HOT Article

- 11. Panagiotopoulos, A. Z. and Yue, S. Dynamics of aqueous electrolyte solutions Challenges for simulations. *The Journal of Physical Chemistry B.* 2023. 127, 2, 430-437. [link]
- Mondal, A., Kussainova, D., Yue, S., and Panagiotopoulos, A. Z. Modeling chemical reactions in alkali carbonate-hydroxide electrolytes with deep learning potentials. *Journal of Chemical Theory* and Computation. 2022. 19, 14, 4584-4595. [link]
  - JCTC Machine Learning for Molecular Simulation Special Issue
- Yue, S., Riera, M.\*, Ghosh, R.\*, Panagiotopoulos, A. Z., and Paesani, F. Transferability of data-driven, many-body models for CO<sub>2</sub> simulations in the vapor and liquid phases. *The Journal of Chemical Physics.* 2022. 156, 104530. [link]
- 8. 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]

- Featured in Springer Nature Research Communities

- Computation and Machine Learning for Chemistry Collection
- 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. *The Journal of Chemical Physics.* 2021. 154, 211103. [link]
  - Featured in JCP Scilight
  - Selected as JCP Featured Article
- Yue, S.\*, Muniz, M. C.\*, Andrade, M. F. C., Zhang, L., Car, R., and Panagiotopoulos, A. Z. When do short-range atomistic machine-learning models fall short? *The Journal of Chemical Physics*. 2021. 154, 034111. [link]
  - Selected as JCP Featured Article

- Kussainova, D., Mondal, A., Young, J. M., Yue, S., and Panagiotopoulos, A. Z. Molecular simulation of liquid-vapor coexistence for NaCl: Full-charge vs scaled-charge interaction models. *The Journal of Chemical Physics.* 2020. 153, 024501. [link]
- Yue, S. and 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]
- 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., and 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]
- 2. Yue, S., Roveda, J. D., Mittenthal, M. S., Shannon, M. S., and 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]
- Fang, Z., Both, J., Li, S., Yue, S., Aprà, E., Keçeli, M., Wagner, A. F., and 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

## GRANTS AND COMPUTATIONAL RESOURCES

PI, NSF ACCESS, "Uncovering structure-property relationships of interfacial electrolytes	2024
using Machine Learning interatomic potentials."	
Co-PI, Cornell-NUS Global Strategic Collaboration Award, "Machine learning for	2024
revealing decisive factors in microwave-assisted pyrolysis of biomass and plastic wastes."	
<b>PI, NSF ACCESS</b> , "Uncovering structure-property relationships in ionic liquid electrolytes using Machine Learning potentials."	2023
<b>Co-PI, NSF XSEDE</b> , "Developing accurate materials design strategies across method- and length-scales." PI: Heather J. Kulik.	2022
<b>Contributor, DOE INCITE</b> , "Multi-scale, ab initio dynamical simulations of heterogeneous electrochemical aqueous interfaces." PI: Roberto Car.	2021
<b>Contributor, DOE BES-CSGB NERSC</b> , "Computational Chemical Science Center: Chemistry in Solution and at Interfaces." PI: Roberto Car.	2020
TEACHING	

Instructor, CHEME 6130: Advanced Chemical Engineering	Fall 2023 – Present
Thermodynamics, Cornell	
Instructor, i-CoMSE Summer School: Machine Learning for Molecular Sci	iences, July 2024
University of Minnesota [link]	
Guest Lecturer, CHEME 7740/5540: Principles of Molecular Simulation,	February 2024
Cornell	
Teaching Assistant, CBE 442 Design, Synthesis, and Optimization of Cher	mical 2017
Processes, Princeton	
Instructor, Honors Seminar on Professional Development, University of Alab	bama Fall 2015

#### STUDENTS MENTORED

Graduate Students:	
Nupur Mehra – PhD student, Cornell CBE	$2023 - \mathrm{Present}$
Spencer Sabatino – PhD student, Cornell CBE	$2023-\mathrm{Present}$
Rahul Sheshanarayana – MS student, Cornell CBE	$2023 - \mathrm{Present}$
Aditi Seshadri – PhD student, Cornell CBE	$2024 - \mathrm{Present}$

Undergraduate Students:	
Anthony Dee, Cornell CBE '25	$2023 - \mathrm{Present}$
Anant Gupta, Cornell CBE '25	$2023-\mathrm{Present}$
Zachary Kwon, Cornell CBE '25	2023 - Present
Nhi Nguyen, Cornell CBE '25	2023 - Present
Prior to Cornell:	
Akash Ball – ChemE PhD student, MIT	Spring 2023
Changhwan Oh – DMSE PhD student, MIT	2022 - 2023
Rafael Chavez – MIT Energy Initiative UROP, MIT	Summer 2022
Maria Muniz – CBE PhD student, Princeton	2019-2021
(currently Associate at McKinsey & Co.)	
Reha Mathur – CBE undergraduate, Princeton	Summer 2021
Andre Guest – CBE Senior Thesis student, Princeton	Fall 2020
Dina Kussainova – Undergraduate summer researcher, Princeton	Summer 2019
(currently PhD student at Princeton)	
Ayanna Matthews – Physics Junior Thesis student, Princeton	Spring 2019
(currently PhD student at UChicago)	

# ACADEMIC AND PROFESSIONAL SERVICE

Organizational and editorial leadership Early Career Board, Journal of Chemical Theory and Computation (JCTC) [link] Early Career Representative, AAAS Section M Engineering [link] Student Research Council Chair, DOE Center for Enhanced Nanofluidic Transport (CENT) EFRC [link]	2024 - 2025 2024 2022 - 2023
Conference/Workshop organization and service	
Session Co-Chair, AIChE 2024: Faculty Candidates in CoMSEF/Area 1A	2024
Instructor, i-CoMSE Summer School 2024: Machine Learning for Molecular Sciences [link]	2024
Reviewer, NeurIPS 2023 AI4Science Workshop [link]	2023
Reviewer, NeurIPS 2023 Generative AI & Biology Workshop [link]	2023
Conference Co-Chair, GRS Chemistry and Physics of Liquids 2023 [link]	2023
Discussion Leader, GRC Chemistry and Physics of Liquids 2023 [link]	2023
Session Chair, AIChE 2022: Innovations in Methods of Data Science	2022
Session Co-Host, Molecular Simulations with Machine Learning Workshop	2020
Session Chair, ACS Fall 2019: Computational Studies of Water	2019

Journal Reviewer: Science Advances, Nature Communications, Chemical Science, Digital Discovery, Journal of Chemical Theory and Computation, Journal of Chemical Physics, Journal of Physical Chemistry, Industrial & Engineering Chemistry Research, Journal of Materials Research

**Proposal Reviewer:** NSF CBET, NSF CDS&E, NSF GRFP, ETH Zürich/Swiss National Supercomputing Centre, Cornell Institute for Digital Agriculture (CIDA)

#### Professional Memberships: AIChE, ACS, AAAS

PhD Thesis committee member:	
June-Yo Chen (Advisor: Yong Joo, Cornell CBE)	$2023 - \mathrm{Present}$
Hongjin Du (Advisor: Julia Dshemuchadse, Cornell MSE)	2023 - Present
Kaushik Chivukula (Advisor: Yu Zhong, Cornell MSE)	2023 - Present
San Lin Htun (Advisor: Jillian Goldfarb, Cornell BEE)	2023 - Present

Departmental Service: Graduate Field Committee Postdoc Committee 2024 CBE Symposium judge	2023 – Present 2023 – Present February 2024
OUTREACH ACTIVITIES	
Field Session Faculty, CATALYST Academy, Cornell Diversity Programs in Engineerin (DPE) [link]	ng July 2024
Field Session Faculty, CURIE Academy, Cornell DPE [link]	July 2024
Faculty Discussion Leader, Cornell DPE Bridge Scholars Program Dinner	November 2023
<ul> <li>Secretary/Treasurer, Princeton Graduate Women in Science and Engineering (GWiSE)</li> <li>Developed programs to advocate for inclusion and gender equality in STEM fields at Prince</li> </ul>	2018 – 2020 aceton.
<b>President, Princeton Graduate Engineering Council</b> Led a 10-member leadership council which served as the liaison between the graduate stu School of Engineering and Applied Science (SEAS) administration, organized SEAS-wide development and social events, managed budget of \$15,000/year.	2017 - 2019 dent body and
<b>Co-lead, Princeton CBE Grad Student Recruitment Team</b> Organized activities and communications for prospective CBE graduate students.	2017, 2018
Mentor, NYC Girls Computer Science and Engineering Conference Mentored 9th and 10th grade girls in NYC high schools to improve their computer scienc provide career advising, helped organize conference as a part of Princeton GWiSE. [about	
<b>President, U. Alabama Student Chapter of the American Chemical Society</b> Led organization to be named the 2015 Most Outstanding Academic Organization at The Alabama, 2015 Honorable Mention for ACS Student Chapter Award by the national ACS Chapter Board.	0
Founder and Director, The 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 $\sim$ 30 student and staff volunteers to carry out project. [press]	
<b>Co-founder and Co-director, STEM Career Exploration Initiative</b> Co-led an extensive 3-week service project to teach math and physics concepts to a 12th g Engineering Applications class at Francis Marion High School in Marion, AL to instill int related fields and provide career advising. Awarded \$800 grant from the University of Ala College to carry out project.	erest in STEM
PRESENTATIONS	
35. Yue, S. Title TBD. ( <i>Invited talk</i> ). Telluride workshop: Multi-Scale Quantum Mechan Condensed Phase Systems: Methods and Applications, July 2024.	nical Analysis of

- 34. Yue, S., Nandy, A., and Kulik, H. J. Discovering molecular coordination environments for selective ion binding using machine learning. (*talk*). AIChE Annual Meeting, November 2023.
- 33. Yue, S. Molecular modeling of ion transport and binding in aqueous electrolyte solutions. (*talk*). Cornell Scientific Computing and Numerics (SCAN) seminar, October 2023.
- 32. Yue, S., Nandy, A., and Kulik, H. J. Discovering molecular coordination environments for selective ion binding using machine learning. (*poster*). Gordon Research Conferences Chemistry and Physics of Liquids, August 2023.

- Yue, S., Nandy, A., and Kulik, H. J. Designing molecular coordination environments for selective ion binding using machine learning. (*poster*). MolSSI Workshop: Machine Learning and Chemistry, May 2023.
- Yue, S., Nandy, A., and Kulik, H. J. Designing molecular coordination environments for selective ion binding using machine learning. (*Invited talk*). Statistical Thermodynamics and Molecular Simulations (STMS) Seminar Series, April 2023. [YouTube video]
- 29. Yue, S., Nandy, A., and Kulik, H. J. Machine-learning enabled design of MOFs for ion-selective membranes. (*talk*). AIChE Annual Meeting, November 2022.
- Yue, S., Muniz, M. C., Andrade, M. F. C., Zhang, L., Car, R., Panagiotopoulos, A. Z. Specific ion effects in aqueous electrolyte solutions from first-principles derived machine-learning potentials. (*invited talk*). Lennard-Jones Centre Discussion Group, The University of Cambridge, October 2022. [YouTube video]
- Yue, S., Nandy, A., Oh, C., Terrones, G., and Kulik, H. J. Ion selectivity and molecular transport in metal-organic frameworks. (*talk*). DOE Center for Enhanced Nanofluidic Transport (CENT), September 2022.
- 26. Yue, S., Nandy, A., Oh, C., Terrones, G., and Kulik, H. J. *In silico* discovery of MOFs for selective ion separation. (*talk*). 2022 MIT Sustainability Conference, MIT J-WAFS, September 2022.
- Yue, S., Nandy, A., Oh, C., Terrones, G., and Kulik, H. J. Modeling fluids in MOFs and CNTs. (*invited talk*) MIT 10.981 Seminar in Colloid and Interface Science (D. Blankschtein group), September 2022.
- Yue, S., Nandy, A., and Kulik, H. J. Machine-learning enabled design of MOFs for ion-selective membranes. (*poster*) Foundations of Molecular Modeling and Simulation (FOMMS), July 2022. (*Received Best Poster Award.*)
- 23. 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.
- 22. Yue, S., Muniz, M. C., Andrade, M. F. C., Zhang, L., Car, R., Panagiotopoulos, A. Z. Thermodynamic and transport properties of aqueous electrolyte solutions: From empirical force fields to machine-learning models. (*talk*) DOE Center for Enhanced Nanofluidic Transport (CENT) Seminar, October 2021.
- Yue, S., Muniz, M. C., Andrade, M. F. C., Zhang, L., Car, R., Panagiotopoulos, A. Z. Designing atomistic machine-learning models for water and electrolyte solutions. (*Invited talk*) Princeton Graduate Certificate in Computational Science and Engineering Colloquium, May 2021.
- 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]
- 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.
- 18. Yue, S., Muniz, M. C., Andrade, M. F. C., Zhang, L., Car, R., Panagiotopoulos, A. Z. Dynamic properties of aqueous electrolyte solutions from nonpolarizable, polarizable, and scaled-charge models & Handling long-range interactions in atomistic machine-learning models. (*talk*) Center for Chemistry in Solution and Interfaces (CSI), Princeton University. October 2020.
- 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*) Merck Award Symposium, Fall 2020 ACS National Meeting. August 2020.
- 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 Environmental Institute Hack Award Symposium. May 2020.

- 15. 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. (*poster*) Andlinger Center for Energy and the Environment 2019 Annual Meeting. November 2019.
- 14. 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*)
- Yue, S. and Panagiotopoulos, A. Z. Dynamic Properties of Aqueous Electrolyte Solutions from Non-Polarizable, Polarizable, and Scaled-Charge Models. (*talk*) Fall 2019 ACS National Meeting. August 2019.
- Yue, S. and Panagiotopoulos, A. Z. Influence of Polarizability on Specific Ion Effects in Aqueous Electrolyte Solution Dynamics. (*poster*) Gordon Research Conference: Chemistry and Physics of Liquids. August 2019.
- 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.
- 10. Yue, S. and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Princeton Research Day. May 2019.
- 9. Yue, S. and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Scientista Symposium. March 2019.
- 8. 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.
- 7. Yue, S. and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Princeton PRISM Poster Session. March 2019.
- Yue, S. and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Andlinger Center for Energy and the Environment 2019 Annual Meeting. November 2018.
- 5. Yue, S. and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Princeton CBE Graduate Student Symposium. October 2018.
- 4. Yue, S. and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Gordon Research Conference: Water and Aqueous Solutions. August 2018.
- 3. Yue, S. and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Gordon Research Seminar: Water and Aqueous Solutions. July 2018.
- 2. Yue, S. and Panagiotopoulos, A. Z. Computational study of ion-water interactions in aqueous electrolyte solutions. (*poster*) Andlinger E-ffiliates Retreat. June 2018.
- 1. Yue, S. and Panagiotopoulos, A. Z. Salt: The secret ingredient to nature's phenamena. (*poster*) Princeton Research Day. May 2018.