SHUWEN YUE

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EDUCATION / TRAINING

Massachusetts Institute of Technology, Cambridge, MA　　　　　　　2021 – 2023
Postdoctoral Research Associate, Department of Chemical Engineering
Advisor: Heather J. Kulik

Princeton University, Princeton, NJ　　　　　　　　　　　　　　　2016 – 2021
Ph.D. in Chemical and Biological Engineering
Certificate in Computational Science and Engineering
Advisor: Athanassios Z. Panagiotopoulos

The University of Alabama, Tuscaloosa, AL　　　　　　　　　　　　2012 – 2016
B.S. in Chemical Engineering and Chemistry
Minor in Mathematics and Computer-based Honors
Advisors: David A. Dixon, Jason E. Bara, Martin A. Bakker

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

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 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, Natural Sciences, Division, The University of Alabama Undergraduate Research and Creative Activity Conference	2014 – 2016
1st place, Physical and Analytical Chemistry Division, Southeastern Undergraduate Research Conference	2015
Dr. Charles L. Seebeck Endowed Scholarship, The University of Alabama	2015
Computer-Based Honors Program Outstanding Sophomore Award, The University of Alabama	2014
1st Place, Alabama Institute for Manufacturing Excellence Student Prototype Competition, The University of Alabama	2014

PUBLICATIONS

17. **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

16. 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

15. 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]

14. 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_2. *The Journal of Physical Chemistry B.* **2023.** 127, 20, 4562–4569. [link]

13. 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 MIT News

12. **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]

10. 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

9. **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. *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

7. 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

6. **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

5. 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]

4. **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]

3. 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]

1. 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

PUBLICATIONS SUBMITTED / IN PREPARATION

1. **Yue, S.**, Car, R., and Panagiotopoulos, A. Z. Role of long-range interactions in atomistic machine-learning potentials of aqueous electrolyte solutions. *In prep.*

GRANTS AND RESOURCES

1. **Co-PI**, Cornell-NUS Global Strategic Collaboration Award, "Machine learning for revealing decisive factors in microwave-assisted pyrolysis of biomass and plastic wastes." (2024)

2. **PI**, NSF ACCESS, "Uncovering structure-property relationships in ionic liquid electrolytes using Machine Learning potentials." (2023)

3. **Co-PI**, NSF XSEDE, "Developing accurate materials design strategies across method- and length-scales." PI: Heather J. Kulik. (2022)

4. **Contributor**, DOE INCITE, "Multi-scale, ab initio dynamical simulations of heterogeneous electrochemical aqueous interfaces." PI: Roberto Car. (2021)

5. **Contributor**, DOE BES-CSGB NERSC, "Computational Chemical Science Center: Chemistry in Solution and at Interfaces" PI: Roberto Car. (2020)

TEACHING EXPERIENCE

Instructor, CHEME 6130: Advanced Chemical Engineering Thermodynamics, Cornell	Fall 2023 – Present
Teaching Assistant, CBE 442 Design, Synthesis, and Optimization of Chemical Processes, Princeton	2017
Instructor, University Honors Seminar on Professional Development, The University of Alabama	Fall 2015

STUDENTS MENTORED

Graduate Students:

Nupur Mehra – PhD student, Cornell CBE	2023 – Present
Spencer Sabatino – PhD student, Cornell CBE	2023 – Present
Rahul Sheshanarayana – MS student, Cornell CBE	2023 – Present
Aditi Seshadri – PhD student, Cornell CBE	2024 – Present

Undergraduate Students:

Anthony Dee, Cornell CBE '25	2023 – Present
Anant Gupta, Cornell CBE '25	2023 – 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)	2024 – 2025
Student Research Council Chair, DOE Center for Enhanced Nanofluidic Transport (CENT) EFRC	2022 – 2023

Conference organization and service

Reviewer, NeurIPS 2023 AI4Science Workshop	2023
Reviewer, NeurIPS 2023 Generative AI & Biology Workshop	2023
Conference Co-Chair, GRS Chemistry and Physics of Liquids 2023	2019 – 2023
Discussion Leader, GRC Chemistry and Physics of Liquids 2023	August 2023
Session Chair, AIChE 2022: Innovations in Methods of Data Science	November 2022
Session Co-Host, Molecular Simulations with Machine Learning Workshop	July 2020
Session Chair, ACS Fall 2019: Computational Studies of Water	August 2019

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

Proposal Reviewer: NSF DMR, NSF GRFP, ETH Zurich/Swiss National Supercomputing Centre

Professional Memberships: AIChE, ACS, AAAS

PhD Thesis committee member:

June-Yu Chen (Advisor: Yong Joo, Cornell CBE)	2023 – 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

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 Grad Student Recruitment Team 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, helped organize conference as a part of Princeton GWiSE [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, 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 ∼30 student and staff volunteers to carry out project [press]

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

PRESENTATIONS

36. **Yue, S.** Title TBD. (*Invited talk*). Telluride workshop: Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications, July 2024.

35. **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.

34. **Yue, S.** Molecular modeling of ion transport and binding in aqueous electrolyte solutions. (*talk*). Cornell Scientific Computing and Numerics (SCAN) seminar, October 2023.

33. **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.

32. **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.

31. **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.

30. **Yue, S.**, Nandy, A., and Kulik, H. J. Machine-learning enabled design of MOFs for ion-selective membranes. (*talk*). AIChE Annual Meeting, November 2022.

29. **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]

28. **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.

27. **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.

26. **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.

25. Nandy, A., **Yue, S.**, Oh, C., and Kulik, H. J. Using Machine-learning, data mining, and experimental data to design ultrastable metal-organic frameworks. (*poster*). MIT Portugal Program Annual Conference, September 2022.

24. **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.

21. **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.

20. **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]

19. **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.

17. **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.

16. **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*)

13. **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.

12. **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.

11. **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.

6. **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.