





# SHUWEN YUE

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## ACADEMIC APPOINTMENTS

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

## EDUCATION / TRAINING

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**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

## AWARDS AND HONORS

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**Scialog Sustainable Minerals, Metals, and Materials (SM3) Fellow and Awardee**, 2024  
Research Corporation for Science Advancement (RCSA)

**Affinito-Stewart Grant**, Cornell PCCW 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 (UA) 2016

**Alexander Stanton Undergraduate Research Award**, UA 2016

**Outstanding Chemistry Undergraduate Research Award**, UA 2016

**Randall Outstanding Undergraduate Research Award**, UA 2014 – 2016

**Natural Sciences Division Award**, UA Undergraduate Research and Creative Activity Conference 2014 – 2016

**1st place, Physical and Analytical Chemistry Division**, Southeastern Undergraduate 2015

**Dr. Charles L. Seebeck Endowed Scholarship**, UA 2015

## PUBLICATIONS

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20. Oh, C., Nandy, A., **Yue, S.**, and Kulik, H. J. MOFs with the Stability for Practical Gas Adsorption Applications Require New Design Rules. *ACS Applied Materials & Interfaces*. **2024**. 16, 41, 55541–55554. [[link](#)]
19. Burton, H., Dong, S., Ghosh, S., Gu, B., Jackson, N., Keefer, D., Lu, Y., Monroe, J., Peng, B., Pieri, E., Spackman, P., Vacher, M., Vuckovic, S., Williams-Young, D., Yang, Z., **Yue, S.**, Zerbe, G., Zhu, T. Editorial: JCTC Early Career Board Selects. *Journal of Chemical Theory and Computation*. **2024**. 20, 14, 5785–5787. [[link](#)]
18. Terrones, G. G., Huang, S.-P., Rivera, M., **Yue, S.**, Hernandez, A., and Kulik, H. J. Metal-organic framework stability in water and harsh environments from data-driven models trained on the diverse WS24 data set. **2024**. 146, 29, 20333–20348. *Journal of the American Chemical Society*. [[link](#)]
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 in Physical Chemistry 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<sub>2</sub>. *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<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

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

## GRANTS AND COMPUTATIONAL RESOURCES

<b>Co-PI</b> , Scialog SM3 Award, Alfred P. Sloan Foundation	2024 – 2025
<b>PI</b> , Affinito-Stewart Grant, Cornell	2024 – 2025
<b>PI</b> , NSF ACCESS	2023 – 2025
<b>Co-PI</b> , Cornell-NUS Global Strategic Collaboration Award	2024
<b>Co-PI</b> , NSF XSEDE (PI: Heather J. Kulik)	2022
<b>Contributor</b> , DOE INCITE (PI: Roberto Car)	2021
<b>Contributor</b> , DOE NERSC (PI: Roberto Car)	2020

## TEACHING

<b>Instructor</b> , CHEME 6130: Advanced Chemical Engineering Thermodynamics, Cornell	Fall 2023, 2024
<b>Instructor</b> , CHEME 3320: Analysis of Separation Processes, Cornell	Spring 2025
<b>Instructor</b> , ENGRG 1050: Engineering Seminar, Cornell	Fall 2024
<b>Instructor</b> , i-CoMSE Summer School: Machine Learning for Molecular Sciences, University of Minnesota <a href="#">[link]</a>	July 2024
<b>Guest Lecturer</b> , CHEME 7740/5540: Principles of Molecular Simulation, Cornell	February 2024
<b>Teaching Assistant</b> , CBE 442 Design, Synthesis, and Optimization of Chemical Processes, Princeton	2017

## ACADEMIC AND PROFESSIONAL SERVICE

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### Organizational and editorial leadership

Liaison Director, AIChE Computational Molecular Science and Engineering Forum (CoMSEF)	2024 – 2026
Early Career Board, Journal of Chemical Theory and Computation (JCTC) <a href="#">[link]</a>	2024 – 2026
Early Career Representative, AAAS Section M Engineering Steering Committee <a href="#">[link]</a>	2024 – 2025
Student Research Council Chair, DOE Center for Enhanced Nanofluidic Transport (CENT) EFRC <a href="#">[link]</a>	2022 – 2023

### Conference/Workshop organization and service

Invited participant, NSF Future of AI in the Mathematical and Physical Sciences (AI+MPS) Workshop	2025
Session Co-Chair, AIChE Faculty Candidates in CoMSEF/Area 1A	2024, 2025
Session Co-Chair, AIChE CoMSEF Poster Session	2025
Poster Judge, ACS COMP / NVIDIA Poster Session	2024
Session Chair, Foundations in Molecular Modeling and Simulation (FOMMS) 2024: Advances in Molecular Modeling and Simulation (MMS)	2024
Reviewer, NeurIPS 2023 AI4Science Workshop	2023
Reviewer, NeurIPS 2023 Generative AI & Biology Workshop	2023
Chair, Gordon Research Seminar, Chemistry and Physics of Liquids	2023
Discussion Leader, Gordon Research Conference, Chemistry and Physics of Liquids	2023
Session Chair, AIChE 2022 Innovations in Methods of Data Science	2022
Session Co-Host, Princeton CSI Molecular Simulations with Machine Learning Workshop	2020
Session Chair, ACS Fall 2019 Computational Studies of Water	2019

**Journal Reviewer:** *Nature Communications, Science Advances, Chemical Science, npj Computational Materials, 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:** DOE BES, NSF CBET, NSF CDS&E, NSF GRFP, ACS PRF, ETH Zürich/Swiss National Supercomputing Centre, Cornell Institute for Digital Agriculture (CIDA), Cornell Global Hubs

**Professional Memberships:** AIChE, ACS, AAAS

### PhD Thesis committee member/examiner:

Junji Zhang (Advisor: Tim Duignan, University of Queensland, Australia)	2024
Katherine Wang (Advisor: Julia Dshemuchadse, Cornell MSE)	2024 – Present
June-Yo 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

### Departmental Service:

Executive Committee	2024 – Present
Graduate Field Committee	2023 – Present
Postdoc Committee	2023 – Present
2024 CBE Symposium judge	February 2024

## TRAINEES SUPERVISED

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### Postdocs:

Osman Mamun	2024 – Present
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### Graduate Students:

Chenlu Yang – PhD student, Cornell CCB	2025 – Present
Aditi Seshadri – PhD student, Cornell CBE	2024 – Present
– NSF GRFP	
Nupur Mehra – PhD student, Cornell CBE	2023 – 2024
Rahul Sheshanarayana – MS student, Cornell CBE	2023 – 2024
Spencer Sabatino – PhD student, Cornell CBE	2023 – 2024

### Undergraduate Students:

Anthony Dee, Cornell CBE '25	2023 – Present
Anant Gupta, Cornell CBE '25	2023 – Present
– Cornell ELI undergraduate research grant	
Zachary Kwon, Cornell CBE '25	2023 – Present
Nhi Nguyen, Cornell CBE '25	2023 – Present
– Cornell ELI undergraduate research grant	
Lyndon Hess, Cornell CCB & Mathematics '27	2024 – Present
James Chen, Cornell CBE '26	2025 – Present

### Before 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
– now Associate at McKinsey	
Reha Mathur – CBE undergraduate, Princeton	Summer 2021
– now Investor at Dimension Capital	
Andre Guest – CBE Senior Thesis student, Princeton	Fall 2020
Dina Kussainova – Undergraduate summer researcher, Princeton	Summer 2019
– now PhD student at Princeton	
Ayanna Matthews – Physics Junior Thesis student, Princeton	Spring 2019
– now PhD student at UChicago	

## INVITED TALKS

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### *At Cornell:*

12. PacifiChem 2025: Challenges in water: From fundamental chemistry to technical applications, Honolulu, HI, December 2025.
11. MRS Fall Meeting 2025: Accelerating Material Research Beyond Data-Driven Approaches – Physical Knowledge and Human Intervention in Autonomous Experiments, Boston, MA. December 2025.
10. AIChE Annual Meeting 2025, CoMSEF: Special Session in Honor of Prof. Thanos Panagiotopoulos 65th Birthday, Boston, MA. November 2025.
9. ACS Fall National Meeting 2025, PHYS: Rare Event Sampling in Material Science Problems: From Fundamental Understanding to Technological Applications, Washington DC, August 2025.
8. Gordon Research Conference: Chemistry and Physics of Liquids, Holderness, NH. August 2025.
7. Cornell University Department of Biological and Environmental Engineering Seminar, Ithaca, NY. December 2024.
6. Cornell University Department of Material Science and Engineering Seminar, Ithaca, NY. November 2024.
5. AIChE Annual Meeting 2024, CoMSEF: Spotlights in Thermodynamics and Computational Molecular Science, San Diego, CA. October 2024.

4. University of Delaware Department of Chemical and Biomolecular Engineering Seminar, Newark, DE. October 2024.
3. ACS Fall National Meeting 2024, I&EC: Data Analytics and AI for Manufacturing and Healthcare, Denver, CO. August 2024.
2. Telluride workshop: Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications, Telluride, CO. July 2024.
1. Cornell Scientific Computing and Numerics (SCAN) Seminar, Ithaca, NY. October 2023.

*Before Cornell:*

6. Statistical Thermodynamics and Molecular Simulations (STMS) Seminar Series (virtual). April 2023. [\[YouTube video\]](#)
5. Lennard-Jones Centre Discussion Group, The University of Cambridge (virtual). October 2022. [\[YouTube video\]](#)
4. MIT 10.981 Seminar in Colloid and Interface Science (D. Blankschtein group), (virtual). September 2022.
3. Women ExceLLing in COmputational Molecular Engineering (WELCOME) Seminar (virtual). November 2020.
2. WCC/Merck Award Symposium, ACS Fall 2020 National Meeting, (virtual). August 2020.
1. Gordon Research Seminar: Chemistry and Physics of Liquids, Holderness, NH. July 2019.

## SELECTED CONTRIBUTED TALKS

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6. ACS COMP: Machine Learning in Chemistry, ACS Fall 2024 National Meeting, Denver, CO. August 2024.
5. MIT Sustainability Conference, MIT J-WAFS, Cambridge, MA. September 2022.
4. Foundations of Molecular Modeling and Simulation (FOMMS), Delavan, WI. July 2022. *Received Best Poster Award.*
3. AIChE Annual Meeting (virtual). November 2020. [\[YouTube video\]](#)
2. Princeton Environmental Institute Hack Award Symposium (virtual). May 2020.
1. Princeton CBE Graduate Student Symposium, Princeton, NJ. October 2019. *Awarded Best Talk in Computational Modeling session.*

## OUTREACH ACTIVITIES

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<b>Panelist</b> , Cornell CBE Women Annual Event	April 2025
<b>Field Session Faculty</b> , CATALYST Academy, Cornell Diversity Programs in Engineering (DPE) <a href="#">[about]</a>	July 2024
<b>Field Session Faculty</b> , CURIE Academy, Cornell DPE <a href="#">[about]</a>	July 2024
<b>Guest Speaker</b> , Cornell SWE Alumni and Faculty Dinner	April 2024
<b>Guest Speaker</b> , Cornell CBE Postdoc Lunch with Faculty	April 2024
<b>Guest Speaker</b> , Cornell CBE WOMEN Lunch with Faculty	April 2024
<b>Guest Speaker</b> , Cornell DPE Bridge Scholars Program Dinner	November 2023
<b>Secretary/Treasurer</b> , Princeton Graduate Women in Science and Engineering (GWiSE)	2018 – 2020
<b>President</b> , Princeton Graduate Engineering Council	2017 – 2019

<b>Co-lead</b> , Princeton CBE Grad Student Recruitment Team	2017, 2018
<b>Mentor</b> , NYC Girls Computer Science and Engineering Conference [ <a href="#">about</a> ]	November 2018
<b>President</b> , U. Alabama Student Chapter of the American Chemical Society	2014 – 2016
<b>Founder and Director</b> , The Greener Tide Project Recycling Initiative [ <a href="#">about</a> ]	2015 – 2016
<b>Co-founder and Co-director</b> , STEM Career Exploration Initiative outreach at Marion High School in Marion, AL	Summer 2013