SHUWEN YUE

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ACADEMIC APPOINTMENTS

Cornell University, Ithaca, NY — July 2023 – Present

Assistant Professor, Robert F. Smith School of Chemical and Biomolecular Engineering

Field Faculty, Materials Science and Engineering

Field Faculty, Mechanical Engineering

Field Faculty, Biological and Environmental Engineering

Faculty Fellow, Cornell Atkinson Center for Sustainability

Affiliate Faculty, Cornell AI for Science Institute

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

AWARDS AND HONORS

Scialog Sustainable Minerals, Metals, and Materials (SM3) Fellow and Awardee, Research Corporation for Science Advancement (RCSA) and Alfred P. Sloan Foundation — 2024, 2025
Affinito-Stewart Grant, Cornell — 2024
Cornell-NUS Global Strategic Collaboration Award, Cornell — 2023
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
1st place, Physical and Analytical Chemistry Division, Southeastern Undergraduate Research Conference — 2015
Dr. Charles L. Seebeck Endowed Scholarship, UA — 2015

PUBLICATIONS

26. Seshadri, A., Hess, L. T. M., and **Yue, S.** Exploring the deviation from Nernst–Einstein conductivity in ionic liquids using machine learning. **2025.** *Submitted.*

25. Ferguson, A., LaFleur, M., Ruthotto, L., Thaler, J., Ting, Y.-S., Tiwary, P., Villanueva-Domingo, P., . . . , **Yue, S.**, et al. The Future of Artificial Intelligence and the Mathematical and Physical Sciences (AI+MPS). **2025.** [preprint]

24. Hess, L. T. M., Nguyen, N. P. T., Dee, A. H., Gupta, A. K., Kwon, Z., and **Yue, S.** How surface functionalization controls confined electrolyte structure and dynamics at graphene interfaces. **2025.** *Submitted.* [preprint]

    – JPCB Athanassios Z. Panagiotopoulos Festschrift

23. Mamun, O. Yang, C. and **Yue, S.** Deep graph kernel learning for material and atomic level uncertainty quantification in adsorption energy prediction. **2025.** *Submitted.* [preprint]

22. Schwindt, N. S., Epsztein, R., Straub, A. P., **Yue, S.**, and Shirts, M. R. Molecular details and free energy barriers of ion de–coordination at elevated salinity and pressure and their consequences for membrane separation. *Journal of Membrane Science.* **2025.** 734, 124358. [link]

21. Ball, A. K., Terrones, G. G., **Yue, S.**, and Kulik, H. J., Data-driven discovery of water-stable metal-organic frameworks with high water uptake capacity. *ACS Applied Materials & Interfaces.* **2025.** 17, 24, 35971–35985. [link]

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.**, Zerze, 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_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

GRANTS AND COMPUTATIONAL RESOURCES

PI, Scialog SM3 Award, Alfred P. Sloan Foundation 2024 – 2025

PI, Affinito-Stewart Grant, Cornell 2024 – 2025

PI, NSF ACCESS compute allocation 2023 – 2026

Co-PI, Cornell-NUS Global Strategic Collaboration Award 2024

Co-PI, NSF XSEDE compute allocation (PI: Heather J. Kulik) 2022

Contributor, DOE INCITE compute allocation (PI: Roberto Car) 2021

Contributor, DOE NERSC compute allocation (PI: Roberto Car) 2020

TEACHING

Instructor, CHEME 6130: Advanced Chemical Engineering Thermodynamics, Cornell 2023 – Present

Instructor, CHEME 3320: Analysis of Separation Processes, Cornell 2025 – Present

Instructor, Institute of Computational Molecular Science Education (i-CoMSE) Summer School: Machine Learning for Molecules [link] 2024, 2025

Instructor, ENGRG 1050: Engineering Seminar, Cornell Fall 2024

Guest Lecturer, CHEME 7740/5540: Principles of Molecular Simulation, Cornell February 2024

Teaching Assistant, CBE 442 Design, Synthesis, and Optimization of Chemical Processes, Princeton 2017

ACADEMIC AND PROFESSIONAL SERVICE

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) 2024 – 2026

Early Career Representative, AAAS Section M Engineering Steering Committee 2024 – 2025

Student Research Council Chair, DOE Center for Enhanced Nanofluidic Transport (CENT) EFRC 2022 – 2023

Conference/Workshop organization and service

Lead Organizer, CECAM Workshop on Physics-aware Machine Learning for Molecules and Materials 2026

Discussion Leader, Gordon Research Conference, Water and Aqueous Solutions 2026

Panelist, Gordon Research Seminar, Water and Aqueous Solutions 2026

Session Co-Chair, AIChE Faculty Candidates in CoMSEF/Area 1A 2024, 2025

Session Co-Chair, AIChE CoMSEF Poster Session 2025

Session Chair, ACS PHYS Rare Events: Machine Learning, Theory, and Mechanisms 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

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*

Workshop Reviewer: NeurIPS 2023 AI4Science Workshop, NeurIPS 2023/2024 Generative AI & Biology Workshop

Proposal Reviewer: DOE BES, NSF DMREF, 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:

Vinamr Jain (Advisor: Fengqi You, Cornell SYSEN)	2025 – Present
Wenhao Yuan (Advisor: Fengqi You, Cornell SYSEN)	2025 – Present
Junji Zhang (Advisor: Tim Duignan, University of Queensland, Australia)	2025
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

Postdocs:

Md Masuduzzaman	2025 – Present
Osman Mamun	2024 – Present

Graduate Students:

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

Undergraduate Students:

Lyndon Hess, Cornell CCB & Mathematics '27	2024 – Present
Anthony Dee, Cornell CBE '25 → Capital One	2023 – 2025
– CBE Outstanding Research by an Undergraduate Award	
Anant Gupta, Cornell CBE '25 → Proctor & Gamble	2023 – 2025
– Cornell ELI undergraduate research grant	
Zachary Kwon, Cornell CBE '25	2023 – 2025
Nhi Nguyen, Cornell CBE '25 → PhD student at MIT ChemE	2023 – 2025
– AIChE Undergraduate Scholarship Award	
– Cornell ELI undergraduate research grant	

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

INVITED TALKS

At Cornell:

13. Pacifichem 2025, Challenges in Water – From Fundamental Chemistry to Technical Applications, Honolulu, HI. December 2025.
12. MRS Fall Meeting 2025, Accelerating Material Research Beyond Data-Driven Approaches – Physical Knowledge and Human Intervention in Autonomous Experiments, Boston, MA. December 2025.
11. AIChE Annual Meeting 2025, CoMSEF – Special Session in Honor of Prof. Thanos Panagiotopoulos 65th Birthday, Boston, MA. November 2025.
10. ACS Fall National Meeting 2025, PHYS: Rare Event Sampling in Material Science Problems – From Fundamental Understanding to Technological Applications, Washington DC. August 2025.
9. Gordon Research Conference: Chemistry and Physics of Liquids, Holderness, NH. August 2025.
8. NSF Future of AI in the Mathematical and Physical Sciences (AI+MPS) Workshop, Cambridge, MA. March 2025.
7. Cornell University Department of Biological and Environmental Engineering Seminar, Ithaca, NY. December 2024. (Field Seminar)
6. Cornell University Department of Material Science and Engineering Seminar, Ithaca, NY. November 2024. (Field Seminar)
5. AIChE Annual Meeting 2024, 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:

7. Statistical Thermodynamics and Molecular Simulations (STMS) Seminar Series (virtual). April 2023. [YouTube video]
6. Lennard-Jones Centre Discussion Group, The University of Cambridge (virtual). October 2022. [YouTube video]

5. MIT 10.981 Seminar in Colloid and Interface Science (D. Blankschtein group) (virtual). September 2022.
4. Women ExceLling in COmputational Molecular Engineering (WELCOME) Seminar (virtual). November 2020.
3. WCC/Merck Award Symposium, ACS Fall 2020 National Meeting (virtual). August 2020.
2. Hack Award Symposium, Princeton Environmental Institute (virtual). May 2020.
1. Gordon Research Seminar: Chemistry and Physics of Liquids, Holderness, NH. July 2019.

SELECTED CONTRIBUTED TALKS

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

OUTREACH ACTIVITIES

Field Session Lead, CATALYST/CURIE Academy, Cornell Engineering High School Outreach Program [about] — 2024, 2025

Panelist, Cornell CBE Women Annual Event — April 2025

Guest Speaker, Cornell SWE Alumni and Faculty Dinner — April 2024

Guest Speaker, Cornell CBE Postdoc Lunch with Faculty — April 2024

Guest Speaker, Cornell CBE WOMEN Lunch with Faculty — April 2024

Guest Speaker, Cornell Bridge Scholars Program — November 2023

Secretary/Treasurer, Princeton Graduate Women in Science and Engineering (GWiSE) — 2018 – 2020

President, Princeton Graduate Engineering Council — 2017 – 2019

Co-lead, Princeton CBE Grad Student Recruitment Team — 2017, 2018

President, U. Alabama Student Chapter of the American Chemical Society — 2014 – 2016

Founder and Director, The Greener Tide Project Recycling Initiative — 2015 – 2016

Co-founder and Co-director, STEM Career Exploration Initiative outreach at Marion High School in Marion, AL — Summer 2013