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
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
Advisors: David A. Dixon, Jason E. Bara, Martin A. Bakker

AWARDS AND HONORS

Affinito-Stewart Grant, Cornell PCCW	2024
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 (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 Research Conference	2015
Dr. Charles L. Seebeck Endowed Scholarship, UA	2015
Computer-Based Honors Program Outstanding Sophomore Award, UA	2014

PUBLICATIONS

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.** [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, Affinito-Stewart Grant, Cornell	2024
PI, NSF ACCESS	2023–2025
Co-PI, Cornell-NUS Global Strategic Collaboration Award	2024
Co-PI, NSF XSEDE (PI: Heather J. Kulik)	2022
Contributor, DOE INCITE (PI: Roberto Car)	2021
Contributor, DOE NERSC (PI: Roberto Car)	2020

TEACHING

Instructor, CHEME 6130: Advanced Chemical Engineering Thermodynamics, Cornell	Fall 2023 – Present
Instructor, ENGRG 1050: Engineering Seminar, Cornell	Fall 2024
Instructor, i-CoMSE Summer School: Machine Learning for Molecular Sciences, University of Minnesota [link]	July 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
Instructor, Honors Seminar on Professional Development, University of Alabama	Fall 2015

ACADEMIC AND PROFESSIONAL SERVICE

Organizational and editorial leadership

Early Career Board, Journal of Chemical Theory and Computation (JCTC) [link]	2024 – 2025
Early Career Representative, AAAS Section M Engineering Steering Committee [link]	2024
Student Research Council Chair, DOE Center for Enhanced Nanofluidic Transport (CENT) EFRC [link]	2022 – 2023

Conference/Workshop organization and service

Session Co-Chair, AIChE 2024: Faculty Candidates in CoMSEF/Area 1A	2024
Poster Judge, ACS COMP / NVIDIA	2024
Session Chair, FOMMS 2024: Advances in MMS	2024
Reviewer, NeurIPS 2023 AI4Science Workshop	2023
Reviewer, NeurIPS 2023 Generative AI & Biology Workshop	2023
Conference Co-Chair, GRS Chemistry and Physics of Liquids	2023
Discussion Leader, GRC Chemistry and Physics of Liquids	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: *Nature Communications*, *Science Advances*, *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: DOE BES, NSF CBET, NSF CDS&E, NSF GRFP, ACS PRF, ETH Zürich/Swiss National Supercomputing Centre, Cornell Institute for Digital Agriculture (CIDA)

Professional Memberships: AIChE, ACS, AAAS

PhD Thesis committee member:

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:

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

TRAINEES SUPERVISED

Postdocs:

Osman Mamun	2024 – Present

Graduate Students:

Nupur Mehra – PhD student, Cornell CBE	2023 – Present
– FOMMS Travel Award and selected for Lightning Talk	
Aditi Seshadri – PhD student, Cornell CBE	2024 – Present
– NSF GRFP	
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

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 & 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
– now PhD student at Princeton	
Ayanna Matthews – Physics Junior Thesis student, Princeton	Spring 2019
– now PhD student at UChicago	

OUTREACH ACTIVITIES

Field Session Faculty, CATALYST Academy, Cornell Diversity Programs in Engineering (DPE) [about]	July 2024
Field Session Faculty, CURIE Academy, Cornell DPE [about]	July 2024
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 DPE Bridge Scholars Program Dinner	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
Mentor, NYC Girls Computer Science and Engineering Conference [about]	November 2018
President, U. Alabama Student Chapter of the American Chemical Society	2014 – 2016
Founder and Director, The Greener Tide Project Recycling Initiative [about]	2015 – 2016
Co-founder and Co-director, STEM Career Exploration Initiative outreach at Marion High School in Marion, AL	Summer 2013

INVITED TALKS

At Cornell:

8. Pacifichem 2025: Challenges in water: From fundamental chemistry to technical applications, Honolulu, HI, December 2025.

7. GRC Chemistry and Physics of Liquids, Holderness, NH. July 2025.

6. Cornell University Department of Material Science and Engineering Seminar, Ithaca, NY. November 2024.

5. Spotlights in Thermodynamics and Computational Molecular Science, AIChE Annual Meeting, San Diego, CA. October 2024.

4. University of Delaware Department of Chemical and Biomolecular Engineering Seminar, Newark, DE. October 2024.

3. ACS I&EC: Data Analytics and AI for Manufacturing and Healthcare, ACS Fall 2024 National Meeting, 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. Fall 2020 ACS National Meeting, (virtual). August 2020.

1. Gordon Research Seminar: Chemistry and Physics of Liquids, Holderness, NH. July 2019.

SELECTED CONTRIBUTED TALKS

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.*