

# SHUWEN YUE

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## ACADEMIC APPOINTMENTS

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<b>Cornell University</b> , Ithaca, NY	July 2023 – Present
<i>Assistant Professor</i> , Robert F. Smith School of Chemical and Biomolecular Engineering	
<i>Field Faculty</i> , Materials Science and Engineering	
<i>Field Faculty</i> , Mechanical Engineering	
<i>Field Faculty</i> , Biological and Environmental Engineering	
<i>Faculty Fellow</i> , Cornell Atkinson Center for Sustainability	
<i>Affiliate Faculty</i> , Cornell AI for Science Institute	

## EDUCATION / TRAINING

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

## AWARDS AND HONORS

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<b>SPROUT Award</b> , Cornell Engineering	2025
<b>Scialog Sustainable Minerals, Metals, and Materials (SM3) Fellow and Awardee</b> , Research Corporation for Science Advancement (RCSA) and Alfred P. Sloan Foundation	2024, 2025
<b>Affinito-Stewart Grant</b> , Cornell	2024
<b>Cornell-NUS Global Strategic Collaboration Award</b> , Cornell	2023
<b>Best Poster Award</b> , Foundations of Molecular Modeling and Simulation (FOMMS)	2022
<b>Early Career Research Award Travel Grant</b> , FOMMS	2022
<b>Princeton nominee for the Schmidt Science Fellowship</b>	2021
<b>WIC Travel Award</b> , The American Institute of Chemical Engineers	2020
<b>WCC Merck Award</b> , The American Chemical Society	2020
<b>Best Talk in Computational Modeling</b> , Princeton CBE Graduate Student Symposium	2019
<b>Mary and Randall Hack '69 Graduate Award</b> , Princeton	2019
<b>Andlinger Center for Energy and the Environment Travel Grant</b> , Princeton	2019
<b>William R. Schowalter Travel Grant</b> , Princeton	2018, 2019
<b>School of Engineering and Applied Science Travel Grant</b> , Princeton	2018
<b>Francis Robbins Upton Fellowship</b> , Princeton	2016 – 2021
<b>Tau Beta Pi Fellowship</b>	2016
<b>Tau Beta Pi Scholarship</b>	2015
<b>Catherine J. Randall Premier Award</b> , The University of Alabama (UA)	2016
<b>Alexander Stanton Undergraduate Research Award</b> , UA	2016
<b>Outstanding Chemistry Undergraduate Research Award</b> , UA	2016
<b>Randall Outstanding Undergraduate Research Award</b> , UA	2014 – 2016

## PUBLICATIONS

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(\*=graduate student, ‡=postdoc, §=undergraduate, †=corresponding author, ¶=equal contributions)

28. Roh, H., Bagatelle, S., **Yue, S.**, **Seshadri, A.**\*, Oh, C., Kulik, H. J., Gumyusenge, A. Diazirine-based crosslinking of amorphous organic ionic-electronic conductors for thermochemical stability in electrochemical devices. **2026.** *In Review.*

27. Villaescusa-Navarro, F., Bolliet, B., Villanueva-Domingo, P., Bayer, A. E., ..., **Mamun, O.**‡, **Yue, S.**, et al. The Denario Project: Modular automation of scientific research with multi-agent systems. **2025.** [\[preprint\]](#)

- Featured in [Simons Foundation News](#)

26. **Seshadri, A.**\*, **Hess, L. T. M.**§, and **Yue, S.**† Exploring the deviation from Nernst–Einstein conductivity in ionic liquids using machine learning. **2025.** *In Review.* [\[preprint\]](#)

- Digital Discovery Emerging Investigator Collection

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

24. **Mamun, O.**‡, **Yang, C.**\*, and **Yue, S.**† Deep graph kernel learning for material and atomic level uncertainty quantification in adsorption energy prediction. **2025.** *In Review.* [\[preprint\]](#)

23. **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.** *Journal of Physical Chemistry B.* [\[link\]](#)

- JPC-B Athanassios Z. Panagiotopoulos Festschrift

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<sub>2</sub>. *The Journal of Physical Chemistry B.* **2023.** 127, 20, 4562–4569. [\[link\]](#)
  - JPC-B Pablo G. Debenedetti Festschrift
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](#)]

## GRANTS AND COMPUTATIONAL RESOURCES

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<b>PI</b> , Flagship Workshop funding, CECAM	2026
<b>PI</b> , SPROUT Award, Cornell Engineering	2026
<b>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 compute allocation	2023 – 2026
<b>Co-PI</b> , Cornell-NUS Global Strategic Collaboration Award	2024
<b>Co-PI</b> , NSF XSEDE compute allocation (PI: Heather J. Kulik)	2022
<b>Contributor</b> , DOE INCITE compute allocation (PI: Roberto Car)	2021
<b>Contributor</b> , DOE NERSC compute allocation (PI: Roberto Car)	2020

## TEACHING

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<b>Instructor</b> , CHEME 6130: Advanced Chemical Engineering Thermodynamics, Cornell	F23, F24, F25
<b>Instructor</b> , CHEME 3320: Analysis of Separation Processes, Cornell	S25
<b>Instructor</b> , Institute of Computational Molecular Science Education (i-CoMSE) Summer School: Machine Learning for Molecules [ <a href="#">link</a> ]	2024, 2025
<b>Instructor</b> , ENRG 1050: Engineering Seminar, Cornell	F24
<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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<b>Organizational and editorial leadership</b>	
<i>Liaison Director</i> , 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

<i>Lead Organizer, CECAM Workshop on Physics-aware Machine Learning for Molecules and Materials</i>	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
<i>Chair, Gordon Research Seminar, Chemistry and Physics of Liquids</i>	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:** *Chemical Science, Chemistry of Materials, Digital Discovery, Industrial & Engineering Chemistry Research, Journal of the American Chemical Society, Journal of Catalysis, Journal of Chemical Physics, Journal of Chemical Theory & Computation, Journal of Materials Research, Journal of Physical Chemistry, Nature Communications, npj Computational Materials, Science Advances*

**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
Wenhai 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

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### Postdocs:

Md Masuduzzaman	2025 – Present
Osman Mamun	2024 – Present

**Graduate Students:**

Prajwal Ananthanarayana – PhD student, Cornell CAM	2026 – Present
Harshvardhan Singh Deora – PhD student, Cornell CCB	2026 – Present
Utkarsh Dogra – PhD student, Cornell CBE	2026 – Present
Chenlu Yang – PhD student, Cornell CCB	2025 – Present
Aditi Seshadri – PhD student, Cornell CBE	2024 – 2025
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:**

Isabella Thomas, Cornell CBE '29	2025 – Present
– Hunter R. Rawlings III Presidential Research Scholar	
James Chen, Cornell CBE '26	2025 – Present
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 → L'Oréal	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:*

14. University of Arkansas Department of Chemical Engineering Seminar, Fayetteville, AR. April 2026.
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

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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

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<b>Field Session Lead</b> , CATALYST/CURIE Academy, Cornell Engineering High School Outreach Program	[about]	2024, 2025
<b>Panelist</b> , Cornell CBE Women Annual Event		April 2025
<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 Bridge Scholars Program		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>President</b> , U. Alabama Student Chapter of the American Chemical Society		2014 – 2016
<b>Founder and Director</b> , The Greener Tide Project Recycling Initiative		2015 – 2016
<b>Co-founder and Co-director</b> , STEM Career Exploration Initiative outreach at Marion High School in Marion, AL		Summer 2013