





# SHUWEN YUE

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## EDUCATION / TRAINING

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

## ACADEMIC APPOINTMENTS

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<b>Cornell University</b> , Ithaca, NY <i>Assistant Professor</i> , Robert F. Smith School of Chemical and Biomolecular Engineering <i>Affiliate Faculty</i> , Cornell AI for Science Institute	July 2023 – Present
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## AWARDS AND HONORS

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<b>Best Poster Award</b> , Foundations of Molecular Modeling and Simulation (FOMMS)	2022
<b>Early Career Research Award</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	2016
<b>Alexander Stanton Undergraduate Research Award</b> , The University of Alabama	2016
<b>Outstanding Chemistry Undergraduate Research Award</b> , The University of Alabama	2016
<b>2016, 2015, 2014 Randall Outstanding Undergraduate Research Award</b> , The University of Alabama	2014 – 2016
<b>2nd Place in 2016, 2nd Place in 2015, 4th place in 2014, Natural Sciences</b> , Division, The University of Alabama Undergraduate Research and Creative Activity Conference	2014 – 2016
<b>1st place, Physical and Analytical Chemistry Division</b> , Southeastern Undergraduate Research Conference	2015
<b>Dr. Charles L. Seebeck Endowed Scholarship</b> , The University of Alabama	2015
<b>Computer-Based Honors Program Outstanding Sophomore Award</b> , The University of Alabama	2014
<b>1st Place, Alabama Institute for Manufacturing Excellence Student Prototype</b> Competition, The University of Alabama	2014

## PUBLICATIONS

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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](#)]
  - Highlighted 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](#)]
  - Highlighted 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](#)]
  - Highlighted 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. Selected as *Featured Article* and *SciLight*. [[link](#)]
  - Selected as JCP Featured Article and Editor’s Choice
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. Selected as *Featured Article*. [[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

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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

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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

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

## STUDENTS MENTORED

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### 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 (currently Associate at McKinsey & Co.)	2019 – 2021
Reha Mathur – CBE undergraduate, Princeton	Summer 2021
Andre Guest – CBE Senior Thesis student, Princeton	Fall 2020
Dina Kussainova – Undergraduate summer researcher, Princeton (currently PhD student at Princeton)	Summer 2019
Ayanna Matthews – Physics Junior Thesis student, Princeton (currently PhD student at UChicago)	Spring 2019

**ACADEMIC AND PROFESSIONAL SERVICE**

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**Organizational and editorial leadership**

Early Career Board, Journal of Chemical Theory and Computation (JCTC)	2024 – 2025
Student Research Council Chair, <a href="#">DOE Center for Enhanced Nanofluidic Transport (CENT) EFRC</a>	2022 – 2023

**Conference organization and service**

Reviewer, NeurIPS 2023 <a href="#">AI4Science Workshop</a>	2023
Reviewer, NeurIPS 2023 <a href="#">Generative AI &amp; Biology Workshop</a>	2023
Conference Co-Chair, <a href="#">GRS Chemistry and Physics of Liquids 2023</a>	2019 – 2023
Discussion Leader, GRC Chemistry and Physics of Liquids 2023: Liquids in Layers and Early-Career Investigators	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**

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<b>Secretary/Treasurer, Princeton Graduate Women in Science and Engineering (GWiSE)</b>	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, 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

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1. **Yue, S.** Title TBD. (*Invited talk*). Telluride workshop: Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications, July 2024.
2. **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.
3. **Yue, S.** Molecular modeling of ion transport and binding in aqueous electrolyte solutions. (*talk*). Cornell Scientific Computing and Numerics (SCAN) seminar, October 2023.
4. **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.
5. **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.
6. **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.
7. **Yue, S.**, Nandy, A., and Kulik, H. J. Machine-learning enabled design of MOFs for ion-selective membranes. (*talk*). AIChE Annual Meeting, November 2022.
8. **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. [\[YouTube video\]](#)



9. **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.
10. **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.
11. **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.
12. 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.
13. **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.*)
14. **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.
15. **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.
16. **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.
17. **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](#)]
18. **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.
19. **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.
20. **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.
21. **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.
22. **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.
23. **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*)
24. **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.

25. **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.
26. **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.
27. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Princeton Research Day. May 2019.
28. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Scientista Symposium. March 2019.
29. **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.
30. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Princeton PRISM Poster Session. March 2019.
31. **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.
32. **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.
33. **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.
34. **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.
35. **Yue, S.** and Panagiotopoulos, A. Z. Computational study of ion-water interactions in aqueous electrolyte solutions. (*poster*) Andlinger E-affiliates Retreat. June 2018.
36. **Yue, S.** and Panagiotopoulos, A. Z. Salt: The secret ingredient to nature's phenomena. (*poster*) Princeton Research Day. May 2018.