





SHUWEN YUE

348A Olin Hall, Ithaca, NY 14853 | 607-255-0848 | shuwen.yue@cornell.edu |    

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
2016, 2015, 2014 Randall Outstanding Undergraduate Research Award, UA 2014 – 2016
2nd Place in 2016, 2nd Place in 2015, 4th place in 2014, Natural Sciences Division, 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
1st Place, Alabama Institute for Manufacturing Excellence Student Prototype Competition, UA 2014

PUBLICATIONS

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. *Under review*. **2024**. [[preprint](#)]
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 CO₂. *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 CO₂ 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

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 [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
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: *Science Advances*, *Nature Communications*, *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, ETH Zürich/Swiss National Supercomputing Centre, Cornell Institute for Digital Agriculture (CIDA)

Professional Memberships: AIChE, ACS, AAAS

PhD Thesis committee member:

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

GRANTS AND COMPUTATIONAL RESOURCES

PI, Affinito-Steward Grant , “Development of physics-informed machine learning potentials for liquid phase phenomena.”	2024
PI, NSF ACCESS , “Uncovering structure-property relationships of interfacial electrolytes using Machine Learning interatomic potentials.”	2024
Co-PI, Cornell-NUS Global Strategic Collaboration Award , “Machine learning for revealing decisive factors in microwave-assisted pyrolysis of biomass and plastic wastes.”	2024
PI, NSF ACCESS , “Uncovering structure-property relationships in ionic liquid electrolytes using Machine Learning potentials.”	2023
Co-PI, NSF XSEDE , “Developing accurate materials design strategies across method- and length-scales.” PI: Heather J. Kulik.	2022
Contributor, DOE INCITE , “Multi-scale, ab initio dynamical simulations of heterogeneous electrochemical aqueous interfaces.” PI: Roberto Car.	2021
Contributor, DOE BES-CSGB NERSC , “Computational Chemical Science Center: Chemistry in Solution and at Interfaces.” PI: Roberto Car.	2020

TEACHING

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

STUDENTS MENTORED***Graduate Students:***

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

Undergraduate Students:

Anthony Dee, Cornell CBE '25	2023 – Present
Anant Gupta, Cornell CBE '25 – Cornell ELI undergraduate research grant	2023 – Present
Zachary Kwon, Cornell CBE '25	2023 – Present
Nhi Nguyen, Cornell CBE '25	2023 – Present
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 – now 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 – now PhD student at Princeton	Summer 2019
Ayanna Matthews – Physics Junior Thesis student, Princeton – now PhD student at UChicago	Spring 2019

OUTREACH ACTIVITIES

Field Session Faculty , CATALYST Academy, Cornell Diversity Programs in Engineering (DPE) [link]	July 2024
Field Session Faculty , CURIE Academy, Cornell DPE [link]	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 [press]	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:

5. **Yue, S.** GRC Chemistry and Physics of Liquids, Holderness, NH. July 2025.
4. **Yue, S.** Physics-Inspired Machine Learning Potentials for Uncovering Mysteries in Electrolyte Solutions. Spotlights in Thermodynamics and Computational Molecular Science, AIChE Annual Meeting, San Diego, CA. October 2024.
3. **Yue, S.** Confinement effects on electrolyte solution dynamics using machine learning potentials. ACS I&EC: Data Analytics and AI for Manufacturing and Healthcare, ACS Fall 2024 National Meeting, Denver, CO. August 2024.
2. **Yue, S.** Physics-Inspired Machine Learning Potentials for Unraveling Mysteries in Electrolyte Solutions. Telluride workshop: Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications, Telluride, CO. July 2024.
1. **Yue, S.** Molecular modeling of ion transport and binding in aqueous electrolyte solutions. Cornell Scientific Computing and Numerics (SCAN) seminar, Ithaca, NY. October 2023.

Before Cornell:

6. **Yue, S.**, Nandy, A., and Kulik, H. J. Designing molecular coordination environments for selective ion binding using machine learning. Statistical Thermodynamics and Molecular Simulations (STMS) Seminar Series (virtual). April 2023. [[YouTube video](#)]
5. **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. Lennard-Jones Centre Discussion Group, The University of Cambridge (virtual). October 2022. [[YouTube video](#)]
4. **Yue, S.**, Nandy, A., Oh, C., Terrones, G., and Kulik, H. J. Modeling fluids in MOFs and CNTs. MIT 10.981 Seminar in Colloid and Interface Science (D. Blankschtein group), (virtual). September 2022.
3. **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. Women ExceLling in COmputational Molecular Engineering (WELCOME) Seminar (virtual). November 2020.
2. **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. Merck Award Symposium, Fall 2020 ACS National Meeting, (virtual). August 2020.
1. **Yue, S.** and Panagiotopoulos, A. Z. Influence of Polarizability on Specific Ion Effects in Aqueous Electrolyte Solution Dynamics. Gordon Research Seminar: Chemistry and Physics of Liquids, Holderness, NH. July 2019.

CONTRIBUTED TALKS

At Cornell:

1. **Yue, S.** Why classical force fields are unable to predict correct water dynamics in salt solutions. (*talk*). ACS COMP: Machine Learning in Chemistry, ACS Fall 2024 National Meeting, Denver, CO. August 2024.

Before Cornell:

27. **Yue, S.**, Nandy, A., and Kulik, H. J. Discovering molecular coordination environments for selective ion binding using machine learning. (*talk*). AIChE Annual Meeting, Orlando, FL. November 2023.
26. **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, Holderness, NH. August 2023.
25. **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, College Park, MD. May 2023.
24. **Yue, S.**, Nandy, A., and Kulik, H. J. Machine-learning enabled design of MOFs for ion-selective membranes. (*talk*). AIChE Annual Meeting, Phoenix, AR. November 2022.
23. **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) seminar (virtual). September 2022.
22. **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, Cambridge, MA. September 2022.
21. **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), Delavan, WI. July 2022. *Received Best Poster Award.*

20. **Yue, S.**, Panagiotopoulos, A. Z. Specific ion effects in aqueous electrolyte solutions from first principles derived machine-learning potentials. (*talk*) AIChE Annual Meeting, Boston, MA. November 2021.
19. **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 (virtual). October 2021.
18. **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. (*talk*) Princeton Graduate Certificate in Computational Science and Engineering Colloquium (virtual). 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 (virtual). November 2020. [[YouTube video](#)]
16. **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 (virtual). October 2020.
15. **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 (virtual). May 2020.
14. **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, Princeton, NJ. November 2019.
13. **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, Princeton, NJ. October 2019. *Awarded Best Talk in Computational Modeling session.*
12. **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, San Diego, CA. August 2019.
11. **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, Holderness, NH. August 2019.
10. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Princeton Research Day, Princeton, NJ. May 2019.
9. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Scientista Symposium, Boston, MA. March 2019.
8. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*talk*) The University of Alabama Department of Chemical Engineering Seminar, Tuscaloosa, AL. March 2019.
7. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Princeton PRISM Poster Session, Princeton, NJ. March 2019.
6. **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, Princeton, NJ. November 2018.
5. **Yue, S.** and Panagiotopoulos, A. Z. Probing water-ion interactions from dynamic properties of aqueous electrolyte solutions. (*poster*) Princeton CBE Graduate Student Symposium, Princeton, NJ. October 2018.

4. **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, Holderness, NH. August 2018.
3. **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, Holderness, NH. July 2018.
2. **Yue, S.** and Panagiotopoulos, A. Z. Computational study of ion-water interactions in aqueous electrolyte solutions. (*poster*) Andlinger E-filiates Retreat, NYC, NY. June 2018.
1. **Yue, S.** and Panagiotopoulos, A. Z. Salt: The secret ingredient to nature's phenomena. (*poster*) Princeton Research Day, Princeton, NJ. May 2018.