Julia H. Yang, Ph.D.
Assistant Professor, Georgia Tech

jhyang@gatech.edu | (404) 939-6629
LinkedIn: julia-yang
she/her/hers

EDUCATION

University of California, Berkeley — Berkeley, CA
Ph.D. in Materials Science & Engineering — Aug. 2016–May 2022

- Thesis advisor: <u>Prof. Gerbrand Ceder</u>
- Thesis: Computational Understanding of Ionic Systems for Advanced Energy Storage Materials
- Minors: Physics, Statistics

Carnegie Mellon University — Pittsburgh, PA
B.S. in Materials Science & Engineering, additional major in Physics — Aug. 2012–May 2016

- Honors research advisor: <u>Prof. Elias Towe</u>
- Honors project: Thermal Transport in Two-Dimensional Semiconductors

EMPLOYMENT

Georgia Institute of Technology — Atlanta, GA
Assistant Professor, School of Chemical and Biomolecular Engineering — Jan. 2025 - present

Harvard University — Cambridge, MA
Environmental Fellow, Center for the Environment — July 2022 –June 2024
Associate — June 2024 –Dec. 2024

- Advised by: <u>Prof. Boris Kozinsky</u>
- Use density functional theory, computational chemistry, and machine learning to model thermal and electrochemical stability of explicit solvents
- Experimental collaboration with Park group (Columbia University)

Columbia University — New York City, NY
Postdoctoral Fellow, Fu Foundation School of Engineering and Applied Science — July 2022 –Aug. 2022

- Advised by: <u>Prof. Ah-Hyung Alissa Park</u>
- Applied electrochemical methods to study electrodeposition of critical materials in organic solvents

University of California, Berkeley — Berkeley, CA
Graduate Student Researcher, Department of Materials Science & Engineering — Aug. 2016 –May 2022

- Advised by: <u>Prof. Gerbrand Ceder</u>
- Advanced coupled cluster expansion lattice models to study high energy and high power density lithium-ion battery electrodes
- Evaluated phase stability in earth-abundant electrodes using first-principles calculations
- Rationalized origin of systematic error in density functional theory approximations for ionic systems

X (formerly Google X), the Moonshot Factory — Mountain View, CA
AI Resident — May 2021 –Sept 2021

- Advised by: Dr. Alexander Holiday
- Developed machine learning platform to optimize chemical recycling of waste plastics
- 4 filed patents (1 first-author patent)

Johns Hopkins Applied Physics Laboratory Laurel, MD

Technical Aide May 2016 –July 2016

- Performed optical analysis of stray photon emission from discarded field-programmable gate arrays for hardware espionage
- Developed experimental setup used in a NASA mission proposal

Honors & Awards

- **NextProf Nexus** at Georgia Institute of Technology — Aug. 2023
- Harvard University Center for the Environment **Environmental Fellow** — July 2022–July 2024
- National Defense Science and Engineering **Graduate Fellow** — Aug. 2016–Aug. 2019
- Carnegie Mellon University **University Honors** — May 2016
- Carnegie Mellon University **College of Engineering Honors** — May 2016
- Carnegie Mellon University **Senior Leadership Award** — May 2016
- U.C. Berkeley Materials Science & Engineering **Rising Star Scholarship** — Awarded Jan. 2016
- Semiconductor Research Corporation **Undergraduate Fellowship** — Jan. 2014–May 2016
- Tau Beta Pi **Engineering Honors Society** — May 2015

Publications

[1] **J. H. Yang**†, A. W. Ooi, Z. A. H. Goodwin, Y. Xie, J. Ding, S. Falletta, A.-H. A. Park, and B. Kozinsky, "Room-temperature decomposition of the ethaline deep eutectic solvent", *J. Phys. Chem. Lett.*, 2025, in press. DOI: 10.1021/acs.jpclett.4c03645.

[2] R. Jacobs, D. Morgan, S. Attarian, J. Meng, C. Shen, Z. Wu, C. Xie, **J. H. Yang**, N. Artrith, B. Blaiszik, G. Ceder, K. Choudhary, G. Csanyi, B. Deng, R. Drautz, J. Godwin, V. Honavar, O. Isayev, A. Johansson, S. Martiniani, S. P. Ong, I. Poltavsky, K. Schmidt, S. Takamoto, A. Thompson, and J. Westermayr, "A practical guide to machine learning interatomic potentials – status and future", *Current opinion in solid state materials science*, 2025, in press.

[3] Z. A. H. Goodwin, M. B. Wenny, **J. H. Yang**, A. Cepellotti, J. Ding, K. Bystrom, B. R. Duschatko, A. Johansson, L. Sun, S. Batzner, A. Musaelian, J. A. Mason, B. Kozinsky, and N. Molinari, "Transferability and accuracy of ionic liquid simulations with equivariant machine learning interatomic potentials", *The Journal of Physical Chemistry Letters*, vol. 15, no. 30, pp. 7539–7547, 2024, PMID: 39023916. DOI: 10.1021/acs.jpclett.4c01942. eprint: https://doi.org/10.1021/acs.jpclett.4c01942.

[4] **J. H. Yang**† and G. Ceder†, "Activated internetwork pathways in partially-disordered spinel cathode materials with ultrahigh rate performance", *Adv. Energy Mater.*, vol. 13, no. 4, p. 2 202 955, 2023. DOI: 10.1002/aenm.202202955.

[5] Z. Jadidi, **J. H. Yang**, T. Chen, L. Barroso-Luque, and G. Ceder, "Ab-initio study of short-range ordering in vanadium-based disordered rocksalt structures", *J. Mater. Chem. A*, vol. 11, pp. 17 728–17 736, 2023. DOI: 10.1039/D3TA02475J.

[6] R. Kam, K. Jun, L. Barroso-Luque, **J. H. Yang**, F. Xie, and G. Ceder, "Crystal structures and phase stability of the $Li_2S\text{-}P_2S_5$ system from first principles", *Chem. Mater.*, vol. 35, pp. 9111–9126, 21 2023. DOI: 10.1021/acs.chemmater.3c01793.

[7] L. Barroso-Luque, **J. H. Yang**, F. Xie, T. Chen, R. L. Kam, Z. Jadidi, P. Zhong, and G. Ceder, "Smol: A python package for cluster expansions and beyond", *J. Open Source Softw.*, vol. 7, no. 77, p. 4504, 2022. DOI: 10.21105/joss.04504.

[8] L. Barroso-Luque, P. Zhong, **J. H. Yang**, F. Xie, T. Chen, B. Ouyang, and G. Ceder, "Cluster expansions of multicomponent ionic materials: Formalism and methodology", *Phys. Rev. B*, vol. 106, no. 14, p. 144 202, 2022. DOI: 10.1103/PhysRevB.106.144202.

[9] T. Chen, **J. H. Yang**, L. Barroso-Luque, and G. Ceder, "Removing the two-phase transition in spinel $LiMn_2O_4$ through cation disorder", *ACS Energy Lett.*, vol. 8, no. 1, pp. 314–319, 2022. DOI: 10.1021/acsenergylett.2c02141.

[10] **J. H. Yang**, T. Chen, L. Barroso-Luque, Z. Jadidi, and G. Ceder, "Approaches for handling high-dimensional cluster expansions of ionic systems", *npj Comput. Mater.*, vol. 8, no. 1, p. 133, 2022. DOI: 10.1038/s41524-022-00818-3.

[11] L. Barroso-Luque, **J. H. Yang**, and G. Ceder, "Sparse expansions of multicomponent oxide configuration energy using coherency and redundancy", *Phys. Rev. B*, vol. 104, p. 224 203, 22 2021. DOI: 10.1103/PhysRevB.104.224203.

[12] **J. H. Yang**, H. Kim, and G. Ceder, "Insights into Layered Oxide Cathodes for Rechargeable Batteries", *Molecules*, vol. 26, no. 11, 2021. DOI: 10.3390/molecules26113173.

[13] H. Kim, D.-H. Kwon, J. C. Kim, B. Ouyang, H. Kim, **J. H. Yang**, and G. Ceder, "Na+ Redistribution by Electrochemical Na+/K+ Exchange in Layered $Na_xNi_2SbO_6$", *Chem. Mater.*, vol. 32, no. 10, pp. 4312–4323, 2020. DOI: 10.1021/acs.chemmater.0c01152.

[14] J. C. *. Kim, D.-H. *. Kwon, **J. H. Yang***, H. Kim, S.-H. Bo, L. Wu, H. Kim, D.-H. Seo, T. Shi, J. Wang, Y. Zhu, and G. Ceder, "Direct Observation of Alternating Octahedral and Prismatic Sodium Layers in O3-Type Transition Metal Oxides", *Adv. Energy Mater.*, vol. 10, no. 31, p. 2 001 151, 2020. DOI: https://doi.org/10.1002/aenm.202001151.

[15] **J. H. Yang**, D. A. Kitchaev, and G. Ceder, "Rationalizing accurate structure prediction in the meta-GGA SCAN functional", *Phys. Rev. B*, vol. 100, no. 3, p. 35 132, 2019. DOI: 10.1103/PhysRevB.100.035132.

[16] Y. Zhang, D. A. Kitchaev, **J. H. Yang**, T. Chen, S. T. Dacek, R. A. Sarmiento-Pérez, M. A. L. Marques, H. Peng, G. Ceder, J. P. Perdew, and J. Sun, "Efficient first-principles prediction of solid stability: Towards chemical accuracy", *npj Comput. Mater.*, vol. 4, no. 1, p. 9, 2018. DOI: 10.1038/s41524-018-0065-z.

[17] C. F. Brasz, **J. H. Yang**, and C. B. Arnold, "Tilting of adjacent laser-induced liquid jets", *Microfluid. Nanofluid.*, vol. 18, no. 2, pp. 185–197, 2015. DOI: 10.1007/s10404-014-1429-4.

* equal contribution | † corresponding author | 6 first-author | 2 corresponding-author

Patents

[1] **J. H. Yang**, V. Gharakhanyan, T. Gadhiya, and A. Holiday, "Ionic liquid-based depolymerization optimization", U.S. Patent App. 17/967,711, filed Oct. 17, 2022.

[2] T. Gadhiya, F. Shah, N. Vyas, V. Gharakhanyan, **J. H. Yang**, and A. Holiday, "Depolymerization optimization platform", U.S. Patent App. 17/967,723, filed Oct. 17, 2022.

[3] V. Gharakhanyan, **J. H. Yang**, T. Gadhiya, and A. Holiday, "Search for candidate molecules using quantum or thermodynamic simulations and autoencoder", U.S. Patent App. 17/967,704, filed Oct. 17, 2022.

[4] T. Ghadiya, F. Shah, N. Vyas, **J. H. Yang**, V. Gharakhanyan, and A. Holiday, "Molecular structure transformers for property prediction", U.S. Patent App. 17/967,685, filed Oct. 17, 2022.

INVITED ORAL PRESENTATIONS

[1] **J. H. Yang**. "Building clean energy technology solutions *in silico*," Georgia Tech Energy Day, April 23, 2025, Georgia Institute of Technology, Atlanta, GA.

[2] **J. H. Yang**. "Understanding the Potential Energy Surface of Green Solvents Using Machine Learning Interatomic Potentials," Lennard-Jones Center Discussion Group, March 17, 2025, University of Cambridge, Cambridge, United Kingdom (virtual).

[3] **J. H. Yang**. "Molecular Simulations of Reactive, Organic Solvents Using Machine Learning Interatomic Potentials", CECAM workshop on Machine Learning Interatomic Potentials and Accessible Databases, Sept. 9-11, 2024, Grenoble, France.

[4] **J. H. Yang**. Princeton University, Andlinger Center for Energy and the Environment, (2024).

[5] **J. H. Yang**. University of Utah, Department of Chemical Engineering, (2024).

[6] **J. H. Yang**. Washington University in St. Louis, Department of Mechanical Engineering and Materials Science, (2024).

[7] **J. H. Yang**. Dartmouth College, Thayer School of Engineering, (2024).

[8] **J. H. Yang**. Boston University, Department of Mechanical Engineering, (2024).

[9] **J. H. Yang**. University of California, Santa Cruz, Department of Chemistry and Biochemistry, (2024).

[10] **J. H. Yang**. University of Rochester, Department of Mechanical Engineering, (2024).

[11] **J. H. Yang**. Georgia Institute of Technology, School of Chemical and Biomolecular Engineering, (2024).

[12] **J. H. Yang**. University of Notre Dame, Aerospace and Mechanical Engineering, (2024).

[13] **J. H. Yang**. University of Notre Dame, Chemical and Biomolecular Engineering, (2024).

[14] **J. H. Yang**. The University of North Carolina at Chapel Hill, Department of Applied Physical Sciences (2024).

[15] **J. H. Yang**. Virginia Polytechnic Institute and State University (Virginia Tech), Department of Chemistry, (2023).

[16] **J. H. Yang**. "Sustainability Challenges in Energy Storage Materials", SOSV, a global venture capital firm, June 28, 2022, San Francisco, CA.

[17] A. Holiday, **J. H. Yang**, V. Gharakhanyan, and T. Gadhiya. (Presentation title withheld due to non-disclosure agreements.) Google X Techforum, Oct. 12, 2021. Presented virtually.

ORAL PRESENTATIONS

[1] **J. H. Yang**. "Removing the Green from Green Solvents", Center for the Environment, Harvard University, April 16, 2024, Cambridge, MA.

[2] **J. H. Yang**, W.-S. A. Ooi, A.-H. A. Park, and B. Kozinsky, "Assessing thermal decomposition reactions in the ethaline green solvent using machine learned interatomic potentials", ACS Fall Meeting, August 13, 2023, San Francisco, CA.

[3] **J. H. Yang**, W.-S. A. Ooi, K. Bystrom, A.-H. A. Park, and B. Kozinsky, "Computational Optimization of Nickel Metal Recovery from Li-ion Cathodes for a Circular Economy in Energy Storage", MRS Spring Meeting, April 12, 2023, San Francisco, CA.

[4] **J. H. Yang**, K. Bystrom, and B. Kozinsky, "Understanding Metal Ion Interactions in Solvents Using First-Principles and Machine Learning Interatomic Potentials", APS March Meeting, March 6, 2023, Las Vegas, NV.

[5] **J. H. Yang**. "Modeling high-component disordered systems for sustainable energy storage materials." U.C. Berkeley Materials Science and Engineering Spring Seminar, March 10, 2022, Berkeley, CA.

[6] **J. H. Yang** and G. Ceder, "*Ab initio* Modeling of Configurational Disorder in Complex Systems by Combining Machine Learning and Cluster Expansions", MRS Fall Meeting, Nov. 29-Dec. 2, 2021, Cambridge, MA.

[7] **J. H. Yang** and G. Ceder. "Thermodynamics of Spinel-like Cation Partial Ordering in Ultrahigh Power and Energy Density Li-ion Batteries for Fast-Charging Electric Vehicles." PRiME 2020 (ECS, ECSJ, & KECS Joint Meeting), Oct. 4-9, 2020. Presented virtually.

[8] **J. H. Yang**, D. A. Kitchaev, and G. Ceder, "Benchmarking the Structure Selection Performance of the SCAN Functional Relative to PBE and PBE-D3", APS March Meeting, March 4-8, 2019. Boston, MA

[9] **J. H. Yang**, C. F. Brasz, and C. B. Arnold, "Time-resolved Imaging Studies of Adjacent Liquid Jet Formation", APS Division of Fluid Dynamics Meeting, Nov. 24-26, 2013. Pittsburgh, PA.

POSTER PRESENTATIONS

[1] **J. H. Yang**, A. W.-S. Ooi, Z. A. Goodwin, A.-H. A. Park, B. Kozinsky, "Assessing chemical reactions in green solvents using reactive machine learning molecular dynamics", Gordon Research Conference on Batteries, Feb. 25-29, 2024. Ventura, CA.

[2] **J. H. Yang** and G. Ceder, "Modeling high-component, disordered rocksalt (DRX) systems for high-energy density Li-ion rechargeable batteries", Gordon Research Conference on Batteries, Feb. 16-21, 2020. Ventura, CA.

Proposals

- **Harvard University**
  Two-year independent postdoctoral proposal funded by Harvard University Center for the Environment | Award: $170,000. July 2022-July 2024

- **Department of Defense**
  Three-year independent graduate school proposal funded by the NDSEG Fellowship | Award: $90,000. Aug. 2016 -July 2019

- **Semiconductor Research Corporation (SRC)**
  Five-semester independent undergraduate research funded by the SRC Undergraduate Research Opportunity (URO) Program | Award: $10,000. Jan. 2014 -May. 2016

Teaching & Mentoring

- **Instructor |** Georgia Tech Jan. 2025–May 2025
  CHBE 2140 - Chemical Engineering Thermodynamics (undergraduate)

- **Guest lecturer on battery recycling |** Harvard University March 27, 2024
  ESPP 90B: The EV Revolution: Outlook, Environmental Impact, Policy, and Challenges (undergraduate/graduate)

- **Guest lecturer on DFT |** Carnegie Mellon University April 2021
  18-817: Fundamentals of Semiconductors and Nanostructures (graduate)

- **Graduate Student Instructor |** U.C. Berkeley Aug. 2019–Dec. 2019
  MSE–201A: Thermodynamics and Phase Transformations in Solids (graduate)

- **Volunteer instructor |** Berkeley High School Sept. 2016-May 2017
  Berkeley Energy and Resources Collaborative High School Program

- **Course Assistant |** Carnegie Mellon University Sept. 2015–Dec. 2015
  15-112: Fundamentals of Programming (undergraduate)

- **Academic Development Peer Tutor |** Carnegie Mellon University Jan. 2013–May 2016
  All core MSE courses (undergraduate)

- **Research Mentor** 2017–present
  Students mentored:
  Stella McWhorter, ChBE B.S. student, Georgia Tech Jan. 2025–present
  Nicolas Wong, ML Ph.D. student, Georgia Tech Jan. 2025–present
  Xinqiang Rao, ChBE Ph.D. student, Georgia Tech Jan. 2025–present
  Whai-Shin Amanda Ooi, ChemE Ph.D. student, Columbia University July 2022–present
  Zinab Jadidi, MSE Ph.D. student, U.C. Berkeley March 2020–May 2022
  Ronald Kam, MSE Ph.D. student, U.C. Berkeley Materials Science & Engineering Sept. 2021–May 2022
  Ryan Riddle, CS/MBA student, U.C. Berkeley Sept. 2017–May 2018

Service

- **Invited speaker, Power Meal**
  Harvard Undergraduate Clean Energy Group   April 2024
- **Lab Representative**   Nov. 2023
  Undergraduate Research Open House for Harvard freshmen and sophomores
- **Reviewer**   Dec. 2022, Dec. 2023, Dec. 2024
  Harvard Computational Science and Engineering Graduate Admissions
- **Discussion leader**
  ACS Fall 2023 | What to Expect from Graduate School   Aug. 2023
- **Symposium organizer**
  MRS Fall 2025 | Solid-State Batteries   Nov. 2025
- **Session chair**
  ACS Fall 2023 | ACS Division of Computers In Chemistry | Materials Science I   Aug. 2023
  ACS Fall 2023 | ACS Division of Computers In Chemistry | Drug Design   Aug. 2023
  MRS Fall 2021 | Symposium CH04 | Accelerating Materials Characterization,
  Modeling, and Discovery by Physics-Informed Machine Learning   Nov. 2021
- **Reviewer**   Mar. 2022–present
  MRS Energy & Sustainability (1), npj Computational Materials (1), ACS Materials Letters (2), ACS Nano (1), Journal of Chemical Theory and Computation (1), Journal of the American Chemical Society (1), Computational Materials Science (1), Science and Technology of Advanced Materials: Methods (1), Nature Computational Science (1), Advanced Energy Materials (1)
- **Thesis Proposal Committee**   Oct. 2024–present
  Youngsu Shin (Advisor: Paul Kohl)   Oct. 2024
  Hazel Gerber (Advisor: Paul Kohl)   March 2025
  Jin Yu (Advisor: Marta Hatzell)   May 2025