

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

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she/her/hers
updated 8/26/25

EDUCATION

University of California, Berkeley Ph.D. in Materials Science & Engineering Advisor: <u>Prof. Gerbrand Ceder</u> <i>Computational Understanding of Ionic Systems for Advanced Energy Storage Materials</i>	Berkeley, CA Aug. 2016–May 2022
Carnegie Mellon University B.S. in Materials Science & Engineering, add. major in Physics Honors advisor: <u>Prof. Elias Towe</u> <i>Thermal Transport in Two-Dimensional Semiconductors</i>	Pittsburgh, PA Aug. 2012–May 2016

EMPLOYMENT

Georgia Institute of Technology Asst. Professor, School of Chemical and Biomolecular Engineering ML Ph.D. Program Faculty Affiliate Faculty, Georgia Tech Advanced Battery Center	Atlanta, GA Jan. 2025–present
Harvard University Environmental Fellow, Associate Advisor: <u>Prof. Boris Kozinsky</u>	Cambridge, MA July 2022–Dec. 2024
Columbia University Visiting Postdoctoral Fellow Advisor: <u>Prof. Ah-Hyung (Alissa) Park</u>	New York City, NY July 2022–Aug. 2022
University of California, Berkeley Graduate Student Researcher Advisor: <u>Prof. Gerbrand Ceder</u>	Berkeley, CA Aug. 2016–May 2022
X (formerly Google X), the Moonshot Factory AI Resident	Mountain View, CA May 2021–Sept 2021
Johns Hopkins Applied Physics Laboratory Technical Aide	Laurel, MD May 2016–July 2016

HONORS & AWARDS

- | | |
|--|---------------------|
| • Google Research Scholar Program | June 2025 |
| • NextProf Nexus at Georgia Institute of Technology | Aug. 2023 |
| • Harvard University Center for the Environment 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** Jan. 2016
- Semiconductor Research Corporation **Undergraduate Fellowship** Jan. 2014–May 2016
- Tau Beta Pi **Engineering Honors Society** May 2015

PUBLICATIONS

- [1] **J. H. Yang**[†], Xinqiang Rao, and A. W. S. Ooi, “Buried no longer: Recent computational advances in explicit interfacial modeling of lithium-based all-solid-state battery materials”, *Frontiers in Energy Research*, vol. 13, Aug. 2025, ISSN: 2296-598X. DOI: 10.3389/fenrg.2025.1621807.
- [2] **J. H. Yang**[†], A. W. S. 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”, *The Journal of Physical Chemistry Letters*, vol. 16, no. 12, pp. 3039–3046, ISSN: 1948-7185. DOI: 10.1021/acs.jpcclett.4c03645.
- [3] R. Jacobs, D. Morgan, S. Attarian, J. Meng, C. Shen, Z. Wu, C. Y. Xie, **J. H. Yang**, N. Artrith, B. Blaiszik, *et al.*, “A practical guide to machine learning interatomic potentials—status and future”, *Current Opinion in Solid State and Materials Science*, vol. 35, p. 101 214, 2025.
- [4] 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.jpcclett.4c01942. eprint: <https://doi.org/10.1021/acs.jpcclett.4c01942>.
- [5] **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. 2202 955, 2023. DOI: 10.1002/aenm.202202955.
- [6] 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.
- [7] R. Kam, K. Jun, L. Barroso-Luque, **J. H. Yang**, F. Xie, and G. Ceder, “Crystal structures and phase stability of the Li_2S - P_2S_5 system from first principles”, *Chem. Mater.*, vol. 35, pp. 9111–9126, 21 2023. DOI: 10.1021/acs.chemmater.3c01793.
- [8] 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.

- [9] 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.
- [10] 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.
- [11] **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.
- [12] 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.
- [13] **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.
- [14] 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.
- [15] 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. 2001 151, 2020. DOI: <https://doi.org/10.1002/aenm.202001151>.
- [16] **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.
- [17] 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.
- [18] 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 | [Yang Lab member](#)

PATENTS

- [1] V. Gharakhanyan, **J. H. Yang**, T. Gadhiya, and A. Holiday, “Search for candidate molecules using quantum or thermodynamic simulations and autoencoder”, U.S. Patent 12,291,608, granted May 6, 2025.

- [2] T. Ghadiya, F. Shah, N. Vyas, **J. H. Yang**, V. Gharakhanyan, and A. Holiday, “Molecular structure transformers for property prediction”, U.S. Patent 12,378,383, granted Aug. 5, 2025.
- [3] **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.
- [4] 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.

INVITED PRESENTATIONS OR SEMINARS

- [1] **J. H. Yang**. “Accelerating the Design of Battery Materials through Modeling,” 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**. “Challenges and Opportunities in Batteries,” ESPP 90B: The EV Revolution, March 27, 2024, Harvard University, Cambridge, MA.
- [5] **J. H. Yang**. Princeton University, Andlinger Center for Energy and the Environment, (2024).
- [6] **J. H. Yang**. University of Utah, Department of Chemical Engineering, (2024).
- [7] **J. H. Yang**. Washington University in St. Louis, Department of Mechanical Engineering and Materials Science, (2024).
- [8] **J. H. Yang**. Dartmouth College, Thayer School of Engineering, (2024).
- [9] **J. H. Yang**. Boston University, Department of Mechanical Engineering, (2024).
- [10] **J. H. Yang**. University of California, Santa Cruz, Department of Chemistry and Biochemistry, (2024).
- [11] **J. H. Yang**. University of Rochester, Department of Mechanical Engineering, (2024).
- [12] **J. H. Yang**. Georgia Institute of Technology, School of Chemical and Biomolecular Engineering, (2024).

- [13] **J. H. Yang**. University of Notre Dame, Aerospace and Mechanical Engineering, (2024).
- [14] **J. H. Yang**. University of Notre Dame, Chemical and Biomolecular Engineering, (2024).
- [15] **J. H. Yang**. The University of North Carolina at Chapel Hill, Department of Applied Physical Sciences (2024).
- [16] **J. H. Yang**. Virginia Polytechnic Institute and State University (Virginia Tech), Department of Chemistry, (2023).
- [17] **J. H. Yang**. “Sustainability Challenges in Energy Storage Materials”, SOSV, a global venture capital firm, June 28, 2022, San Francisco, CA.
- [18] A. Holiday, **J. H. Yang**, V. Gharakhanyan, and T. Gadhiya. (Presentation title withheld due to non-disclosure agreements.) Google X Techforum, Oct. 12, 2021. Virtual.

SELECT ORAL PRESENTATIONS

- [1] **J. H. Yang**. “Approximating a Dynamic Reaction Pathway in Explicit Solvents Using Machine Learning Interatomic Potentials and Ab Initio Molecular Dynamics”, MRS Fall Meeting, Nov. 30-Dec. 5, 2025, Boston, MA.
- [2] **J. H. Yang**, A. W. S. Ooi, A.-H. A. Park, B. Kozinsky. “Training Lean: New Approaches for Developing Machine Learning Interatomic Potentials for Simulations of Chemical Reactivity in Liquids”, AIChE Annual Meeting, Nov. 2-6, 2025, Boston, MA.
- [3] **J. H. Yang**. “Lessons Learned from Ethaline: Design Principles for Deep Eutectic Solvents”, 248th ECS Meeting, Oct. 14, 2025, Chicago, IL.
- [4] **J. H. Yang**. “Removing the Green from Green Solvents”, Center for the Environment, Harvard University, April 16, 2024, Cambridge, MA.
- [5] **J. H. Yang**, A. W. S. 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.
- [6] **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.
- [7] **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.

- [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

- **Google**
LLM-GUAL | Award: \$60,000. June 2025
- **Harvard University**
Center for the Environment Postdoctoral Fellowship | Award: \$170,000. July 2022
- **Department of Defense**
NDSEG Fellowship | Award: \$90,000. Aug. 2016
- **Semiconductor Research Corporation (SRC)**
SRC Undergraduate Research Opportunity | Award: \$10,000. Jan. 2014

TEACHING

- **CHBE 2140 - Chemical Engineering Thermodynamics** Jan. 2025–May 2025
Instructor, Georgia Tech
Students: 43, Overall effectiveness: 4.87/5
- **MSE-201A: Thermo. and Phase Trans. in Solids** Aug. 2019–Dec. 2019
Graduate Student Instructor, U.C. Berkeley
- **15-112: Fundamentals of Programming** Sept. 2015–Dec. 2015
Course Assistant, Carnegie Mellon University

GRADUATE STUDENTS

- **Nicolas Wong** | Georgia Tech | ML Ph.D. program Jan. 2025–present
- **Xinqiang Rao** | Georgia Tech | ChBE Ph.D. program Jan. 2025–present
- **Shreya Dimri** | Georgia Tech | CS Master’s program Sept. 2025–present

UNDERGRADUATE STUDENTS

- **Stella McWhorter** | Georgia Tech | ChBE B.S. Jan. 2025–present
- **Minji Kyung** | Georgia Tech | ChBE B.S. Sept. 2025–present
- **Callie Marriaga** | Georgia Tech | ChBE B.S. Sept. 2025–present
- **Joongho Sohn** | Georgia Tech | ChBE B.S. Sept. 2025–present
- **Jayda Howard** | Albany State University | Biology B.S. May–June 2025

ACADEMIC SERVICE

- **Symposium organizer**
MRS Fall 2025 | Solid-State Batteries Nov. 2025
ACS Spring 2026 | Battery Recycling March 2026
- **Tutorial organizer**
MRS Fall 2025 | Solid-State Batteries Nov. 2025
- **Reviewer** Dec. 2022, Dec. 2023, Dec. 2024
Harvard Computational Science and Engineering Graduate Admissions
- **Session chair**
ACS Fall 2023 | ACS Division of Computers In Chemistry |
Materials Science I, Drug Design Aug. 2023
MRS Fall 2021 | Accelerating Materials Characterization, Modeling, and
Discovery by Physics-Informed Machine Learning Nov. 2021
- **Reviewer** Mar. 2022–present
MRS Energy & Sustainability, npj Computational Materials, ACS Materials Letters,
ACS Nano, Journal of Chemical Theory and Computation, Journal of the American
Chemical Society, Computational Materials Science, Science and Technology of
Advanced Materials: Methods, Nature Computational Science, Advanced Energy
Materials, Nature Communications
- **Thesis Proposal Committee** Oct. 2024–present
Youngsu Shin (Advisor: Paul Kohl) Oct. 2024
Hazel Gerber (Advisor: Paul Kohl) March 2025
Adam Hsieh (Advisor: Nian Liu) May 2025
Jin Yu (Advisor: Marta Hatzell) June 2025
Andy Chang (Advisor: David Flaherty) Fall 2025

CONSULTING

- **Google**
Visiting Research Faculty Sept.-Dec. 2025

SERVICE AND OUTREACH

- Community-Engaged Sustainability Research **Faculty Fellows Program** 2025-2026
- ChBE Graduate Seminar Series **Committee** Fall 2025
- ChBE Graduate Recruitment Weekend **Committee** Spring 2025, Spring 2026
- **Invited speaker, Power Meal**
Harvard Undergraduate Clean Energy Group April 2024
- **Lab Representative** Nov. 2023
Undergraduate Research Open House for Harvard freshmen and sophomores
- **Discussion leader**
ACS Fall 2023 | What to Expect from Graduate School Aug. 2023
- **Volunteer instructor** | Berkeley High School Sept. 2016-May 2017
Berkeley Energy and Resources Collaborative High School Program