

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

jhyang@gatech.edu | (404) 939-6629  
LinkedIn: julia-yang  
she/her/hers  
updated 6/13/25

## EDUCATION

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<b>University of California, Berkeley</b> 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
<b>Carnegie Mellon University</b> 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

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<b>Georgia Institute of Technology</b> 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
<b>Harvard University</b> Environmental Fellow, Associate Advisor: <u>Prof. Boris Kozinsky</u>	Cambridge, MA July 2022 –Dec. 2024
<b>Columbia University</b> Visiting Postdoctoral Fellow Advisor: <u>Prof. Ah-Hyung (Alissa) Park</u>	New York City, NY July 2022 –Aug. 2022
<b>University of California, Berkeley</b> Graduate Student Researcher Advisor: <u>Prof. Gerbrand Ceder</u>	Berkeley, CA Aug. 2016 –May 2022
<b>X (formerly Google X), the Moonshot Factory</b> AI Resident	Mountain View, CA May 2021 –Sept 2021
<b>Johns Hopkins Applied Physics Laboratory</b> Technical Aide	Laurel, MD May 2016 –July 2016

## HONORS & AWARDS

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| • Google Research Scholar Program                          | May 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

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- [1] **J.H. Yang**<sup>†</sup>, 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, Mar. 2025, ISSN: 1948-7185. DOI: 10.1021/acs.jpcclett.4c03645.
- [2] 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.
- [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.jpcclett.4c01942. eprint: <https://doi.org/10.1021/acs.jpcclett.4c01942>.
- [4] **J.H. Yang**<sup>†</sup> and G. Ceder<sup>†</sup>, “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  $Li_2S$ - $P_2S_5$  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. 2001 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

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- [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 App. 17/967,704, granted May 6, 2025.
- [2] **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.

- [3] 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.
- [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 PRESENTATIONS OR SEMINARS

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- [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

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- [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**. “Modeling high-component disordered systems for sustainable energy storage materials.” U.C. Berkeley Materials Science and Engineering Spring Seminar, March 10, 2022, Berkeley, CA.
- [4] **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.
- [5] **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
- [6] **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

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- [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

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- **Google**  
LLM-GUAL | Award: \$60,000. May 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

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- **CHBE 2140 - Chemical Engineering Thermodynamics** Jan. 2025–May 2025  
*Instructor*, Georgia Tech
- **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

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- **Nicolas Wong** | Georgia Tech | ML Ph.D. program Jan. 2025–present
- **Xinqiang Rao** | Georgia Tech | ChBE Ph.D. program Jan. 2025–present

## UNDERGRADUATE STUDENTS

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

## ACADEMIC SERVICE

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- **Symposium 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

## SERVICE AND OUTREACH

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- **Graduate Seminar Series Committee**  
Georgia Tech ChBE Fall 2025
- **Graduate Recruitment Weekend Committee**  
Georgia Tech ChBE 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