Julia H. Yang, Ph.D.

Environmental Fellow, Harvard University

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(she/her/hers)

Summary

I am a **computational materials scientist** focused on **sustainability** challenges in **energy storage**. My research advances and applies first-principles and machine learning approaches to navigate chemical space and design urgently-needed materials for **energy and the environment**.

Education

Harvard University — Cambridge, MA
Environmental Fellow — July 2022 –present

- Postdoctoral advisor: Prof. Boris Kozinsky
- Independent research proposal funded through Harvard University Center for the Environment

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

- Thesis advisor: Prof. Gerbrand Ceder
- 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: Prof. Elias Towe
- Honors project: Thermal Transport in Two-Dimensional Semiconductors

Experience

Harvard University — Cambridge, MA
Environmental Fellow, John A. Paulson School of Engineering and Applied Sciences — July 2022 –present

- Advised by: Prof. Boris Kozinsky
- 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)
- 4 journal publications in preparation (1 first-author/corresponding author)

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

- Advised by: Prof. Ah-Hyung Alissa Park
- 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: Prof. Gerbrand Ceder

- 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
- 13 journal publications (5 first or co-first author, 1 corresponding author)

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] 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.*, accepted.

[2] **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.

[3] 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*, 2023, Advance Article. DOI: doi.org/10.1039/D3TA02475J.

[4] 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.

[5] 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.

[6] 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.

[7] **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.

[8] 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.

[9] **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.

[10] 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.

[11] 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.

[12] **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.

[13] 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.

[14] 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.

In preparation

- H. Yang, **J. H. Yang**, B. Kozinsky, and J. J. Vlassak, "Complex ion crosslinked on-demand-dissociable chitosan with extended working pH range".
- **J. H. Yang**†, A. W.-S. Ooi, Y. Xie, Z. A. Goodwin, J. Ding, S. Falletta, A.-H. A. Park, and B. Kozinsky†, "Thermal decomposition of the ethaline deep eutectic solvent".
- Z. A. Goodwin, **J. H. Yang**, M. B. Wenny, A. Cepellotti, A. Johansson, L. Sun, S. Batzner, A. Musaelian, J. A. Mason, N. Molinari, and B. Kozinsky, "Chemically accurate ionic liquid simulations via graph neural nets".
- D. Morgan, B. Kozinsky, V. Honavar, *et al.*, "A Practical Guide to Machine Learning Potentials – Status and Future".

* 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, "Depolymerizeration 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] 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.

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

[3] **J. H. Yang**. Atom-by-Atom Design of Sustainable Energy Storage Solutions. Virginia Polytechnic Institute and State University (Virginia Tech), Department of Chemistry Seminar, Dec. 6, 2023, Blacksburg, VA.

[4] **J. H. Yang**. Atom-by-Atom Design of Sustainable Energy Storage Solutions. The University of North Carolina at Chapel Hill, Department of Applied Physical Sciences, Jan. 8, 2024, Chapel Hill, NC.

[5] **J. H. Yang**. Atom-by-Atom Design of Sustainable Energy Storage Solutions. University of Notre Dame, School of Chemical and Biomolecular Engineering, Jan. 15, 2024, Notre Dame, IN.

[6] **J. H. Yang**. Atom-by-Atom Design of Sustainable Energy Storage Solutions. University of Notre Dame, School of Aerospace and Mechanical Engineering, Feb. 13, 2024, Notre Dame, IN.

Oral Presentations

[1] **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.

[2] **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.

[3] **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.

[4] **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.

[5] **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.

[6] **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.

[7] **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

[8] **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** 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.

Teaching & Mentoring

- **Guest lecturer on DFT** | Carnegie Mellon University — April 2021
  18-817: Fundamentals of Semiconductors and Nanostructures (graduate-level)
- **Graduate Student Instructor** | U.C. Berkeley — Aug. 2019–Dec. 2019
  MSE–201A: Thermodynamics and Phase Transformations in Solids (graduate-level)
- **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-level)
- **Academic Development Peer Tutor** | Carnegie Mellon University — Jan. 2013–May 2016
  All core MSE courses (undergraduate-level)
- **Research Mentor** — 2017–present
  Students mentored:
  Whai-Shin Amanda Ooi, Ph.D. student, Columbia University Chemical Engineering — July 2022–present
  Zinab Jadidi, Ph.D. student, U.C. Berkeley Materials Science & Engineering — March 2020–May 2022
  Ronald Kam, Ph.D. student, U.C. Berkeley Materials Science & Engineering — Sept. 2021–May 2022
  Ryan Riddle, Master's student, U.C. Berkeley Computer Science — Sept. 2017–May 2018

Service

- **Session chair**
  MRS Fall 2021 | Symposium CH04 | Accelerating Materials Characterization, Modeling, and Discovery by Physics-Informed Machine Learning — Boston, MA
  ACS Fall 2023 | ACS Division of Computers In Chemistry | Materials Science I — San Francisco, CA
  ACS Fall 2023 | ACS Division of Computers In Chemistry | Drug Design — San Francisco, CA
- **Discussion leader**
  ACS Fall 2023 | What to Expect from Graduate School — San Francisco, CA
- **Reviewer** — Mar. 2022–present
  MRS Energy & Sustainability (1), npj Computational Materials (1), ACS Materials Letters (2)
- **Reviewer** — Jan. 2023
  Harvard SEAS Graduate Admissions
- **Lab Representative** — Nov. 2023
  Undergraduate Research Open House for Harvard freshmen and sophomores

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

Skills

- **Programming:** Python, bash, R
- **Computational:** density functional theory, computational chemistry, Monte Carlo methods, cluster expansion method, molecular dynamics, machine learning interatomic potentials
- **Experimental:** Electrochemical analysis, laser induced forward transfer

References

- **Gerbrand Ceder**
  Samsung Distinguished Chair in Nanoscience and Nanotechnology Research
  Department of Materials Science and Engineering
  University of California, Berkeley
  gceder@berkeley.edu
- **Boris Kozinsky**

Thomas D. Cabot Associate Professor of Computational Materials Science
Harvard John A. Paulson School of Engineering and Applied Sciences
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bkoz@seas.harvard.edu

- **Ah-Hyung Alissa Park**
  Ronald and Valerie Sugar Dean and Professor
  Department of Chemical and Biomolecular Engineering
  University of California, Los Angeles
  apark@seas.ucla.edu
- **Alexander Holiday**
  Senior Machine Learning Engineer
  X, the Moonshot Factory
  Milwaukee, WI
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