

Julia H. Yang, Ph.D.  
Environmental Fellow, Harvard University

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(she/her/hers)

## SUMMARY

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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

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**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

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**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

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- **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

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- [1] **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. 2202955, 2023. DOI: 10.1002/aenm.202202955.
  - [2] 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. 17728–17736, 2023. DOI: 10.1039/D3TA02475J.
  - [3] 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.
  - [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/acseenergylett.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, 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

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- [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

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- [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.

## ORAL PRESENTATIONS

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- [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

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- [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

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- **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

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- **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

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- **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

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- **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

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- **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  
Harvard University  
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  
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- **Alexander Holiday**

Senior Machine Learning Engineer

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