

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

jhyang@g.harvard.edu | (631) 312-7365
Website: juliayang.github.io
(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 Monolayer 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

AI Resident

Mountain View, CA

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

Technical Aide

Laurel, MD

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] 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”, (submitted).
 - [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. 2202955, 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, “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.

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**. “Sustainability Challenges in Energy Storage Materials” (Invited), SOSV, a global venture capital firm, June 28, 2022, San Francisco, CA.
- [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] 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.
- [8] **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.
- [9] **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

- [10] **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:

<u>Whai-Shin Amanda Ooi</u> , Ph.D. student, Columbia University Chemical Engineering	July 2022–present
<u>Zinab Jadidi</u> , Ph.D. student, U.C. Berkeley Materials Science & Engineering	March 2020–May 2022
<u>Ronald Kam</u> , Ph.D. student, U.C. Berkeley Materials Science & Engineering	Sept. 2021–May 2022
<u>Ryan Riddle</u> , 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 Chemisry | Materials Science I San Francisco, CA
ACS Fall 2023 | ACS Division of Computers In Chemisry | 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)

PROPOSALS

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

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