

Jonas L. Kaufman

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Education

University of California, Santa Barbara (UCSB)

Ph.D. Materials

GPA: 4.0

June 2022

Harvey Mudd College (HMC)

B.S. Physics

Graduate with High Distinction, Departmental Honors in Physics and Humanities

GPA: 3.9

May 2017

Experience

Postdoctoral Researcher, Lawrence Livermore National Laboratory

Aug. 2022–Present

Developing computational methods for kinetic simulations of materials for energy applications.

Graduate Student Researcher, Van der Ven Group, UCSB

Sep. 2017–Jun. 2022

Conducted research on thermodynamic and kinetic properties of battery electrode materials using high-throughput electronic structure calculations and statistical mechanics methods. Developed and supported scientific software tools for materials simulation.

Academic Cooperation Participant, Lawrence Livermore National Laboratory

Jun.–Sep. 2019

Performed large-scale molecular dynamics simulations to probe non-equilibrium properties of candidate hydrogen storage materials.

HMC Clinic Team Member, Sandia National Laboratories, Albuquerque

Sep. 2016–May 2017

Led finite element modeling effort to investigate dielectric properties of nanoparticle composites.

Materials Science Research Assistant, UNSW Sydney, Australia

May–Aug. 2015, 2016

Performed atomistic modeling of mechanical properties to aid development of multicomponent metallic alloys.

Awards

Best Oral Presentation Award, Materials Research Society Spring Meeting

2021

U.S. Department of Energy Computational Science Graduate Fellowship

2017–2021

Jon A. Wunderlich Prize for Creative Achievement in Physics, HMC

2017

Barry M. Goldwater Scholarship

2016–2017

Jude and Eileen Laspa Fellowship in Applied Mechanics, HMC

2015–2017

National Merit Scholarship

2013–2017

Publications

Google Scholar profile

13. K. E. Wyckoff, L. Kautzsch, **J. L. Kaufman**, B. R. Ortiz, A. Kallistova, G. Pokharel, J. Liu, K. M. Taddei, K. M. Wiaderek, S. H. Lapidus, S. D. Wilson, A. Van der Ven, and R. Seshadri. [Electrochemical control of magnetism on the breathing kagome network of \$\text{Li}_x\text{ScMo}_3\text{O}_8\$](#) . *Chemistry of Materials* 35, 4945–4954 (2023).
12. B. Puchala, J. C. Thomas, A. R. Natarajan, J. G. Goiri, S. S. Behara, **J. L. Kaufman**, and A. Van der Ven. [CASM — A software package for first-principles based study of multicomponent crystalline solids](#). *Computational Materials Science* 217, 111897 (2023).
11. **J. L. Kaufman** and A. Van der Ven. [First-principles investigation of phase stability in layered \$\text{Na}_x\text{CrO}_2\$](#) . *Physical Review Materials* 6, 115401 (2022).
10. K. E. Wyckoff, **J. L. Kaufman**, S. W. Baek, C. Dolle, J. J. Zak, J. Bienz, L. Kautzsch, R. C. Vincent, A. Zohar, K. A. See, Y. M. Eggeler, L. Pilon, A. Van der Ven, and R. Seshadri. [Metal-metal bonding as an electrode design principle in the low-strain cluster compound \$\text{LiScMo}_3\text{O}_8\$](#) . *Journal of the American Chemical Society* 144, 5841–5854 (2022).
9. **J. L. Kaufman** and A. Van der Ven. [Cation diffusion facilitated by antiphase boundaries in layered intercalation compounds](#). *Chemistry of Materials* 34, 1889–1896 (2022).
8. **J. L. Kaufman** and A. Van der Ven. [Antiphase boundary migration as a diffusion mechanism in a \$\text{P}_3\$ sodium layered oxide](#). *Physical Review Materials* 5, 055401 (2021). Editors' Suggestion.
7. E. Hwang, E. Cuddy, J. Lin, **J. L. Kaufman**, A. Shaw, P. L. J. Conway, A. Pribram-Jones, K. J. Laws, and L. Bassman. [Predicting ductility in quaternary \$\text{B}_2\$ -like alloys](#). *Physical Review Materials* 5, 033604 (2021).
6. **J. L. Kaufman** and A. Van der Ven. [Ordering and structural transformations in layered \$\text{K}_x\text{CrO}_2\$ for K-ion batteries](#). *Chemistry of Materials* 32, 6392–6400 (2020).
5. **J. L. Kaufman**, J. Vinckevičiūtė, S. K. Kolli, J. G. Goiri, and A. Van der Ven. [Understanding intercalation compounds for sodium-ion batteries and beyond](#). *Philosophical Transactions of the Royal Society A* 377, 20190020 (2019).
4. M. Y. Toriyama, **J. L. Kaufman**, and A. Van der Ven. [Potassium ordering and structural phase stability in layered \$\text{K}_x\text{CoO}_2\$](#) . *ACS Applied Energy Materials* 2, 2629–2636 (2019).
3. **J. L. Kaufman** and A. Van der Ven. [\$\text{Na}_x\text{CoO}_2\$ phase stability and hierarchical orderings in the \$\text{O}_3/\text{P}_3\$ structure family](#). *Physical Review Materials* 3, 015402 (2019).
2. **J. L. Kaufman**, S. H. Tan, K. Lau, A. Shah, R. G. Gambee, C. Gage, L. MacIntosh, A. Dato, P. N. Saeta, R. C. Haskell, and T. C. Monson. [Permittivity effects of particle agglomeration in ferroelectric ceramic-epoxy composites using finite element modeling](#). *AIP Advances* 8, 125020 (2018).
1. **J. L. Kaufman**, G. S. Pomrehn, A. Pribram-Jones, R. Mahjoub, M. Ferry, K. J. Laws, and L. Bassman. [Stacking fault energies of nondilute binary alloys using special quasirandom structures](#). *Physical Review B* 95, 094112 (2017).

Presentations

4. **DOE CSGF Program Review.** *First-principles thermodynamics and kinetics of layered intercalation compounds for “beyond Li-ion” batteries*. Jul. 21, 2021. Virtual.
3. **Materials Research Society Spring Meeting.** *Hierarchical intercalant orderings in layered oxides for Na- and K-ion battery electrodes*. Apr. 21, 2021. Virtual. Best Oral Presentation Award.
2. **Gordon Research Conference: Batteries.** *Modeling structural evolution in layered cathode materials for Na- and K-ion batteries*. Poster. Feb. 17–18, 2020. Ventura, CA.
1. **Materials Research Society Spring Meeting.** *Structural phase transitions and intercalant ordering in layered Na- and K-ion cathode materials*. Apr. 23, 2019. Phoenix, AZ.

Teaching & Mentorship

Alumni Research Mentor, HMC Sep. 2017–Present
Advise undergraduate students from various academic backgrounds on applying first-principles techniques to materials research problems.

Materials Teaching Assistant, UCSB Sep.–Dec. 2018
Conducted recitation sections and office hours for *Introduction to Quantum Mechanics for Materials*.

Future Leaders in Advanced Materials Mentor, UCSB May–Sep. 2018
Mentored visiting undergraduate student researcher on project that culminated in a publication.

Physics Academic Excellence Program Facilitator, HMC May 2015–May 2017
Led tutoring workshops for students in Special Relativity, Mechanics, and Electromagnetism courses.