Jonas L. Kaufman

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Education

University of California, Santa Barbara (UCSB)
Ph.D. Materials — June 2022
GPA: 4.0

Harvey Mudd College (HMC)
B.S. Physics — May 2017
Graduate with High Distinction, Departmental Honors in Physics and Humanities
GPA: 3.9

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

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 Na_xCrO_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 $LiScMo_3O_8$. *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 P3 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 B2-like alloys. *Physical Review Materials* 5, 033604 (2021).

6. **J. L. Kaufman** and A. Van der Ven. Ordering and structural transformations in layered K_xCrO_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 K_xCoO_2. *ACS Applied Energy Materials* 2, 2629–2636 (2019).

3. **J. L. Kaufman** and A. Van der Ven. Na_xCoO_2 phase stability and hierarchical orderings in the O3/P3 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.