Jonas L. Kaufman

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Education

University of California, Santa Barbara (UCSB)
Ph.D. Materials — Expected May 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

***Graduate Student Researcher*, Van der Ven Group, UCSB** — Sep. 2017–Present

Materials Science Research
Conduct research on thermodynamic and kinetic properties of battery electrode materials using high-throughput electronic structure calculations and statistical mechanics methods. Provide theoretical insights to experimentalist collaborators developing novel functional materials.

CASM: A Clusters Approach to Statistical Mechanics (https://github.com/prisms-center/CASMcode)
Provide support to group members and external users. Identify and address bugs. Implemented new feature to enable modeling of electronic ordering phenomena, along with unit tests. Wrote plugins for common tasks within casm-utilities, a simplified interface to the CASM C++ library.

kmc-lotto (https://github.com/jonaskaufman/kmc-lotto)
Developed lightweight, open-source C++ library for event selection in arbitrary kinetic Monte Carlo simulations, eventually to be used in CASM. Built custom simulator using kmc-lotto to model unconventional diffusion mechanism.

Python Development
Curate and contribute to collection of Jupyter notebooks illustrating various machine learning approaches to fitting surrogate models to first-principles thermodynamic data. Lead development of package to provide problem-specific functionality for fitting and analysis workflows.

***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. Wrote various Python scripts to set up and monitor simulations, analyze results.

***HMC Clinic Team Member*, Sandia National Laboratories, Albuquerque** — Sep. 2016–May 2017
Led computational modeling effort to investigate dielectric properties of nanoparticle composites. Built COMSOL application with Java backend to easily run simulations and visualize results. Integrated four years of teams' computational results into a publication.

***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

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*. Accepted.

9. **J. L. Kaufman** and A. Van der Ven. Cation diffusion facilitated by antiphase boundaries in layered intercalation compounds. *Chemistry of Materials* (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.

Skills

Programming Languages & Tools
Proficient: C++, C, Python, Bash, Mathematica, MATLAB, Git, Autotools, GoogleTest, pytest
Familiar: Java, Fortran, CUDA, Racket, Prolog

Scientific Computing
Comprehensive practical knowledge of Unix-like systems and high-performance computing clusters
Experience with simulation codes: VASP, Qball, COMSOL

Other
Proficient: LaTeX, Microsoft Office, Inkscape, GIMP