Luis Barroso-Luque, Ph.D.

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SUMMARY

I am a skilled and experienced computational materials scientist with a proven track record of success in developing and applying novel computational methods. I have developed novel computational methods with improved the accuracy, performance and interpretability for inorganic material property predictions. I am also an active contributor to several open-source projects in Python and C/C++, which have been used by thousands of other researchers. I am proficient in a variety of computational techniques, including numerical and simulation methods, statistical inference, machine learning, and data analysis. I am confident that my skills and experience would be a valuable asset to your team.

I am generally interested in the use of high-performance computing, atomistic modeling, data-driven models, and machine learning to tackle pressing theoretical and applied problems in the physical sciences with a focus on energy, environment, and climate applications.

RESEARCH EXPERIENCE

Lawrence Berkeley National Laboratory   Berkeley, CA
Postdoctoral Researcher   Oct. 2022 - Oct. 2023

- Develop, implement, and optimize graph convolutional neural network models for large-scale molecular dynamics simulations.
- Formulate and implement inference and sampling methodology for lattice-based thermodynamic calculations of partially disordered solids.
- Generate and benchmark novel parameterized lattice model construction and Monte Carlo sampling strategies for prediction of ionic conductivity, voltage, and phase stability of cathodes and super-ionic conductors.
- Administration, software installation, and user support for Linux (Debian/Ubuntu) research computing clusters.

University of California, Berkeley   Berkeley, CA
Graduate Student Researcher   Sept. 2016 - Sept. 2022

- Developed and implemented applied lattice model and Monte Carlo sampling methodology to study configurational thermodynamics of metallic alloys, cathodes, and super-ionic conductors.
- Performed high-throughput density functional theory calculations of metal oxides and alloys.
- Implemented novel lattice model parameter estimation with structured sparsity based on regularized linear regression and mixed integer programming.
- Managed and completed three-year grant administration and reporting requirements during award and closure stages.
- Administration, software installation, and user support for Linux (Debian/Ubuntu) research computing clusters.

Advanced Light Source at Lawrence Berkeley National Laboratory   Berkeley, CA
Research Fellow   Sept. 2015 - Aug. 2016

- Developed microtomography image reconstruction and analysis software for the Advanced Light Source synchrotron X-ray source.
- Implemented graphical interface and backend functions for data processing, reconstruction, and analysis of tomographic data in the XI-CAM data analysis interface.
- Implemented integration of Beamline 8.3.2 datasets with standard Python microtomography libraries TOMOPY and DXCHANGE.
- Developed workflow for automatic data processing and tomographical reconstruction on National Energy Research Scientific Computing Center (NERSC) supercomputing system.

OPEN SOURCE PROJECTS

SMOL	Main developer and maintainer of a package for constructing and Monte Carlo sampling of atomic configuration lattice models.
SPARSE-LM	Main developer and maintainer of a package implementing several SCIKIT-LEARN compatible sparse linear regression models.
CHGNET	Contributor to implementation of universal graph neural network potential for charge-informed atomistic modeling of materials.
MATGL	Contributor to a graph deep learning library for materials science
PYMATGEN	Contributor to one of the largest and most widely used materials analysis libraries.
XI-CAM	Contributor to a popular graphical environment for synchrotron data analysis, management, and visualization.
TOMOPY	Contributor to package implementing pre-/post-processing functionality and reconstruction algorithms for hard X-ray tomography.

SKILLS

Programming	Python (NumPy, SciPy, Cython, scikit-learn, cvxpy, PyTorch, matplotlib, plotly), C/C++, Git, Github
Computing	Shell (Bash), MPI, OpenMP, High Performace Computing, MongoDB
Simulation	VASP, Lammps, Mathematica, MATLAB, COMSOL
Miscellaneous	Linux, OS-X, LaTeX, beamer, Markdown, reStructuredtext
Languages	English (professional proficiency), Spanish (native)

EDUCATION

University of California, Berkeley
Berkeley, CA
Ph.D. in Computational Materials Science
Aug. 2016 - Sept. 2022
- Designated Emphasis in Computational and Data Science and Engineering
- Awards: NSF Graduate Research Fellowship (2017-2022); UC Berkeley Chancellor's Fellowship (2016-2018)

Boston University
Boston, MA
B.S. in Mechanical Engineering, *summa cum laude*
Aug. 2012 - Sept. 2015
- Minors in Physics and Mathematics; concentration in Energy Technology; Honors: Tau Beta Pi; Pi Tau Sigma

TEACHING EXPERIENCE

University of California, Berkeley
Berkeley, CA
Guest Lecturer, *Thermodynamics and Phase Transformations in Solids*
Fall 2022
- Presented course lectures on introductory statistical mechanics of non-interacting and weakly interacting systems
- Developed and drafted exam questions.

Graduate Student Instructor, *Thermodynamics and Phase Transformations in Solids*
Fall 2019
- Prepared lecture materials, held office hours, and led recitations relating to thermodynamics and statistical mechanics of solids.
- Developed, drafted, and graded exam questions.

PUBLICATIONS

Ronald L. Kam, KyuJung Jun, **Luis Barroso-Luque**, Julia H. Yang, Fengyu Xie, and Gerbrand Ceder. Crystal Structures and Phase Stability of the Li_2S-P_2S_5 System from First Principles. *(Under review)*. doi:10.48550/arXiv.2307.00878.

Peichen Zhong, Fengyu Xie, **Luis Barroso-Luque**, Liliang Huang, and Gerbrand Ceder. Modeling intercalation chemistry with multi-redox reactions by sparse lattice models in disordered rocksalt cathodes. *(Under review)*. doi:10.48550/arXiv.2307.03717.

Zinab Jadidi, Julia H. Yang, Tina Chen, **Luis Barroso-Luque**, and Gerbrand Ceder. Ab-initio study of short-range ordering in vanadium-based disordered rocksalt structures. *(Under review)*, 2023. doi:10.48550/arXiv.2304.14645.

Luis Barroso-Luque and Gerbrand Ceder. The cluster decomposition of the configurational energy of multicomponent alloys. *(Under review)*, 2023. doi:10.48550/arxiv.2301.02309.

Fengyu Xie, Peichen Zhong, **Luis Barroso-Luque**, Bin Ouyang, and Gerbrand Ceder. Semigrand-canonical Monte-Carlo simulation methods for charge-decorated cluster expansions. *Computational Materials Science*, 218:112000, 2023. doi:10.1016/j.commatsci.2022.112000.

Tina Chen, Julia Yang, **Luis Barroso-Luque**, and Gerbrand Ceder. Removing the Two-Phase Transition in Spinel LiMn2O4 through Cation Disorder. *ACS Energy Letters*, 8(XXX):314–319, 2023. doi:10.1021/acsenergylett.2c02141.

Luis Barroso-Luque, Julia H. Yang, Fengyu Xie, Tina Chen, Ronald L. Kam, Zinab Jadidi, Peichen Zhong, and Gerbrand Ceder. SMOL: A Python package for cluster expansions and beyond. *Journal of Open Source Software*, 7(77):4504, 2022a. ISSN 2475-9066. doi:10.21105/joss.04504.

Luis Barroso-Luque, Peichen Zhong, Julia H. Yang, Fengyu Xie, Tina Chen, Bin Ouyang, and Gerbrand Ceder. Cluster expansions of multicomponent ionic materials: Formalism and methodology. *Physical Review B*, 106(14):144202, 2022b. doi:10.1103/PhysRevB.106.144202.

Peichen Zhong, Tina Chen, **Luis Barroso-Luque**, Fengyu Xie, and Gerbrand Ceder. An $\ell_0\ell_2$-norm regularized regression model for construction of robust cluster expansions in multicomponent systems. *Physical Review B*, 106(2):024203, 2022. doi:10.1103/PhysRevB.106.024203.

Julia H. Yang, Tina Chen, **Luis Barroso-Luque**, Zinab Jadidi, and Gerbrand Ceder. Approaches for handling high-dimensional cluster expansions of ionic systems. *npj Computational Materials*, 8(1):1–11, 2022. ISSN 2057-3960. doi:10.1038/s41524-022-00818-3.

Luis Barroso-Luque, Julia H. Yang, and Gerbrand Ceder. Sparse expansions of multicomponent oxide configuration energy using coherency and redundancy. *Physical Review B*, 104(22):224203, 2021. doi:10.1103/PhysRevB.104.224203.

Qingsong Tu, **Luis Barroso-Luque**, Tan Shi, and Gerbrand Ceder. Electrodeposition and Mechanical Stability at Lithium-Solid Electrolyte Interface during Plating in Solid-State Batteries. *Cell Reports Physical Science*, 1(7):100106, 2020. ISSN 2666-3864. doi:10.1016/j.xcrp.2020.100106.

Luis Barroso-Luque, Qingsong Tu, and Gerbrand Ceder. An Analysis of Solid-State Electrodeposition-Induced Metal Plastic Flow and Predictions of Stress States in Solid Ionic Conductor Defects. *Journal of the Electrochemical Society*, 167(2):020534, 2020. ISSN 1945-7111. doi:10.1149/1945-7111/ab6c5b.

R. J. Pandolfi, D. B. Allan, E. Arenholz, **L. Barroso-Luque**, and et al. Xi-cam: A versatile interface for data visualization and analysis. *Journal of Synchrotron Radiation*, 25(4):1261–1270, 2018. ISSN 1600-5775. doi:10.1107/S1600577518005787.

INTERESTS

Aspiring mountaineer   Climbing, backcountry skiing, overall snow science nerd.

Cycling enthusiast   Mountain biking and road cycling. Nine times out of ten I'd rather bike there.

Arch Linux   I have been on the rolling release bleeding edge of the Linux kernel since I started graduate school.