

Leo J. Beck

Computational Scientist

 Boulder, CO

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 <https://leobbeckportfolio.vercel.app/>

Summary

Ph.D. candidate with a strong math background and extensive experience building data-driven models and scalable compute workflows (**Python, HPC, optimization**).

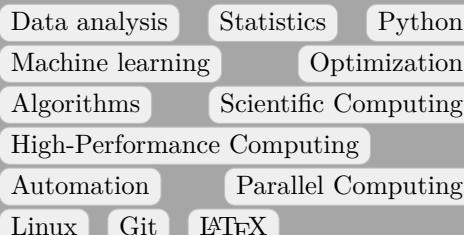
Social Network



<https://github.com/leojbeck>

leo-beck

Core Skills



Tools

-  Python, Excel, C/C++, MATLAB, VBA / Power Automate
-  Valgrind, Intel Advisor, LAMMPS, NAMD, VMD, VASP

Honors

-  Gilbert Robinson Research Award (Clemson, 2023)
-  South Carolina State High School Geography Champion, (2019)

Languages

 English



 German



 Spanish



Experience

Dec 2023 –
Present

Graduate Researcher

University of Colorado Boulder

Built high-throughput simulation / analysis automation tools (Python/bash; Slurm/MPI); ran hybrid perovskite simulations in LAMMPS.

Aggregated structured datasets; engineered features; trained/validated supervised ML models (cross-validation; class-imbalance mitigation; error analysis).

Multiple manuscripts under review.

May 2025 –
Aug 2025

Classical Simulations Consultant

FAIRmat (Berlin, DE)

Extended the NOMAD LAMMPS parser in Python; curated diverse regression test cases; advised on LAMMPS methods/options.

Strengthened robustness for edge cases; documented assumptions and failure modes for maintainable parsing.

May 2024 –
Aug 2024

High-Performance Computing Intern

Air Force Research Lab

Performed replicated LAMMPS shear simulations of $Ti_3C_2T_x$ MXenes; estimated slip probability vs. force and fit logistic curves to extract inter-sheet shear strength.

Automated post-processing/visualization in Python; generated publication-ready figures and summaries.

May 2023 –
Aug 2023

Engineering & Planning Intern

Benore Logistic Systems, Inc.

Built driver-utilization visualization tool and automated daily analytics using VBA and Power Automate; implemented first-fit decreasing algorithm to automate pallet-to-truck packing (VBA).

Improved plan quality and reduced manual effort through automated reporting and repeatable heuristics.

Education

Aug 2023 –
Present

Ph.D. Materials Science & Engineering

University of Colorado Boulder

Aug 2023 –
May 2025

M.S. Materials Science & Engineering

University of Colorado Boulder

GPA: 3.90/4.00

Aug 2019 –
May 2023

B.S. Materials Science & Engineering &

Clemson University

B.S. Mathematics

GPA: 3.84/4.00

Leadership & Teaching

May 2021 –
Jun 2022

Financial & Logistics Officer

Clemson Formula SAE

Increased annual team revenue from school from \$30k to \$70k; managed a \$100k budget and logistics for 30 members.

May 2020 –
May 2023

Head of Procurement / Electrical Division Member

Clemson Formula SAE

Coordinated hundreds of purchase requests across 8 divisions; supported vehicle electrical harness/sensor integration and test days.

Fall 2023,
Spring 2026

Physics Teaching Assistant

University of Colorado Boulder

Led recitations and labs, graded coursework, and proctored exams for General Physics 1, Experimental Physics 1, and Classical Mechanics & Math Methods 1.

Selected Publications

2025

Enhancing Dimensionality Prediction in Hybrid Metal Halides via Feature Engineering and Class-Imbalance Mitigation

Karabin *et Al.*

2025

Validated Reactive Force Field Quantifies Mxene Interfacial Properties, Mechanics, and Thermal Transport

Armstrong *et Al.*