Leo J. Beck

Computational Scientist

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https://leobeckportfolio.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

Data analysis | Statistics | Python | Machine learning | Optimization | Algorithms | Scientific Computing | High-Performance Computing | Automation | Parallel Computing | Linux | Git | LaTeX

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 & B.S. Mathematics**, Clemson University
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.