Janosh Riebesell

Member of Technical Staff, Periodic Labs

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Computational materials scientist working on machine-learning interatomic potentials, high-throughput electronic-structure calculations, and open-source atomistic modeling and analysis software.

Experience

Periodic Labs — Member of Technical Staff

Sep 2025 – present

- Develop high-throughput density functional theory workflows and machine-learning force fields for atomistic simulations.

Radical AI

Apr 2024 – Jun 2025

- Built Radical AI's high-throughput density functional theory pipeline.
- Co-created TorchSim, a PyTorch-native engine for batched atomistic simulations.

Materials Project

Jul 2022 – Dec 2023

- Contributed to CHGNet and MACE-MP foundation models for atomistic simulations.
- Developed high-throughput workflows generating reference datasets for interatomic-potential training.

Selected open source

Matbench Discovery — Maintainer

site · code · 251 stars

- Developed a benchmark evaluating machine-learning models in realistic crystal-discovery campaigns.

TorchSim — Maintainer

site · code · 488 stars

- Co-develop a PyTorch-native engine for batched atomistic simulations.

CHGNet — Maintainer

site · code · 404 stars

- Helped develop a charge-informed interatomic potential.

MACE Foundation Models — Contributor

site · code · 302 stars

- Helped train and evaluate MACE-MP for atomistic simulations.

pymatgen — Maintainer

site · code · 1961 stars

- Python materials-analysis library powering the Materials Project.

atomate2 — Maintainer

code · 347 stars

- Implemented MatPES PBE and r2SCAN workflows generating reference data for universal interatomic potentials.

Publications

* first or joint first author, † senior author

1. * J. George, ..., **J. Riebesell**, ..., S. Ong. pymatgen: 15 years of community growth, new functionality, and future prospects. *preprint* (2026). link
2. M. Horton, ..., **J. Riebesell**, ..., K. Persson. Accelerated data-driven materials science with the Materials Project. *Nature Materials* (2025). link
3. A. Ganose, ..., **J. Riebesell**, ..., A. Jain. Atomate2: modular workflows for materials science. *Digital Discovery* (2025). link
4. * **J. Riebesell**, R. Goodall, ..., K. Persson. Matbench Discovery - A framework to evaluate machine learning crystal stability predictions. *Nature Machine Intelligence* (2025). link
5. A. Kaplan, ..., **J. Riebesell**, ..., S. Ong. A Foundational Potential Energy Surface Dataset for Materials. *preprint* (2025). link
6. B. Deng, ..., **J. Riebesell**, ..., G. Ceder. Systematic softening in universal machine learning interatomic potentials. *npj Computational Materials* (2025). link
7. O. Cohen, **J. Riebesell**, ..., A. Gangan. TorchSim: An efficient atomistic simulation engine in PyTorch. *IOP AI for Science* (2025). link
8. * **J. Riebesell**, T. Surta, ..., A. Lee. Discovery of high-performance dielectric materials with machine-learning-guided search. *Cell Reports Physical Science* (2024). link
9. M. Evans, ..., **J. Riebesell**, ..., R. Armiento. Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange. *Digital Discovery* (2024). link
10. † Y. Chiang, C. Chou, **J. Riebesell**. LLaMP: Large Language Model Made Powerful for High-fidelity Materials Knowledge Retrieval and Distillation. *preprint* (2024). link

11. A. Rosen, ..., **J. Riebesell**, ..., A. Ganose. Jobflow: Computational Workflows Made Simple. *Journal of Open Source Software* (2024). link
12. * I. Batatia, ..., **J. Riebesell**, ..., G. Csányi. A foundation model for atomistic materials chemistry. *arXiv.org* (2023). link
13. B. Deng, ..., **J. Riebesell**, ..., G. Ceder. CHGNet as a pretrained universal neural network potential for charge-informed atomistic modelling. *Nature Machine Intelligence* (2023). link
14. M. Horton, ..., **J. Riebesell**, ..., K. Persson. Crystal Toolkit: A Web App Framework to Improve Usability and Accessibility of Materials Science Research Algorithms. *preprint* (2023). link

Education

PhD in Physics — University of Cambridge

Thesis: Towards Machine Learning Foundation Models for Materials Chemistry

MPhil in Scientific Computing — University of Cambridge

Thesis: Probabilistic Data-Driven Discovery of Thermoelectric Materials

MSc in Physics — ITP Heidelberg

Thesis: Functional Renormalization Group Analytically Continued to Finite Temperatures

BSc in Physics — Hamburg University

Thesis: van der Waals Corrections for Density Functional Theory - DFT+D2 applied to Graphene-hBN-Heterostructures

Skills

Scientific computing	Python Rust PyTorch JAX HPC
Atomistic simulation	VASP Quantum ESPRESSO ASE pymatgen
Tooling	Git Slurm Node.js Deno Vite Playwright
Web	TypeScript Svelte React REST MongoDB

Community

IOP Associate Editor IOP AI for Science · 2025 – present

Reviewer for Nature Computational Science, npj Computational Materials, JACS, JCTC, JMLR, Digital Discovery · 2022 – present

Cambridge Physical Society · 2020 – present

Materials Research Society · 2023 – present

Materials Project Software Foundation · 2023 – present

Languages, nationality and interests

English (advanced), German (native), French (intermediate), Spanish (basic). Canadian and German citizen.

photography hiking cycling climbing