

# SABA KHARABADZE, PHD

sabakharabadze.com | s.kharabadze@gmail.com | linkedin.com/in/kharabadze | Google Scholar

Pisa, Tuscany, Italy

## SUMMARY

ML Research Engineer / Research Scientist with 6+ years building ML-enabled scientific and signal-processing systems. Experienced in GPU/distributed workflows, large-scale data generation and processing (1M+ structures, 1TB data), HPC environments (GPU nodes, job scheduling, software stack installation), and C/C++ + Python ML pipelines (PyTorch/JAX).

## SKILLS

<b>Programming</b>	Python (PyTorch, JAX, NumPy, SciPy, pandas), C/C++, SQL, Bash, Git
<b>Systems/Infra</b>	Docker, Linux, HPC (GPU nodes, schedulers), CUDA, multi-GPU training, distributed training
<b>Scientific/Domain</b>	DFT (VASP, Gaussian), materials modeling, numerical simulation
<b>Languages</b>	English (native/bilingual), Georgian (native/bilingual), Russian (proficient)

## RESEARCH ENGINEERING EXPERIENCE

**ML Research Engineer (Research Scientist) - *CNIT RaSS Lab - Pisa, Italy*** April 2025 - Present

- Build ML-based radar signal processing workflows for target detection.
- Develop simulation frameworks for coverage analysis of mono- and multistatic radar systems.
- Implement reproducible experimentation code and analysis pipelines for model evaluation and system-level studies.

**Physics AI Model Validation Expert - *Handshake MOVE Program - Remote*** August 2025 - Present

- Design physics reasoning problems and reference solutions to stress-test AI model capabilities.
- Evaluate model responses and write targeted feedback to improve reasoning and physics correctness.

**PhD Candidate - *Binghamton University (SUNY) - Binghamton, NY*** August 2018 - August 2024

- Built end-to-end pipelines for ML-accelerated atomistic simulation: data generation, model training, and high-throughput search.
- Scaled evolutionary search + ML potential workflows to **1M+ structures** and **1TB** energy/force data using HPC clusters.
- Developed Python tooling to transform raw simulation outputs into physical/electrochemical/structural properties used for discovery decisions.
- Implemented and validated an **NPT barostat** module in **C** for in-house molecular dynamics software (MAISE); achieved thermal expansion coefficients within 10% of experiment.
- Administered two university HPC clusters (1000+ CPU cores plus GPU nodes): installed/maintained compilers, CUDA, MPI, PyTorch stack, and scientific codes; enabled multi-node and multi-GPU use.

## SELECTED PROJECT HIGHLIGHTS

- **ML-accelerated discovery of Li-Sn phases:** created DFT reference data (VASP), trained/used a neural network potential (C), and executed high-throughput evolutionary searches; identified **8 new stable structures** and validated stability with phonons.
- **Thermodynamic stability of Li-B-C compounds:** computed chemical potentials and performed quasi-harmonic phonon analysis to study stability across volumes and temperatures; published results in PCCP.
- **Engineering for reproducibility:** built scripts, Python tooling and deployed documentation website (Sphinx) for simulation workflows; maintained a public documentation site for MAISE.

EDUCATION

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**PhD in Physics**, Binghamton University, State University of New York May 2024  
Dissertation: Machine Learning and *ab initio* insights into the design of lithium-based materials.

**B.S. in Physics**, Free University of Tbilisi May 2017  
Minor: Computer Science and Mathematics

SELECTED PUBLICATIONS

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- Kharabadze, S. *et al.* (2022) Prediction of stable Li-Sn compounds: boosting ab initio searches with neural network potentials. *npj Comput Mater.*
- Kharabadze, S. *et al.* (2023) Thermodynamic stability of Li-B-C compounds from first principles. *Phys. Chem. Chem. Phys.*
- Hajinazar, S. *et al.* (2021) MAISE: Construction of neural network interatomic models and evolutionary structure optimization. *Comput. Phys. Commun.*

ADDITIONAL INDUSTRY EXPERIENCE

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**Back-end Developer - *Eleven Wireless*** - *Remote (Portland, OR)* Oct 2017 – Apr 2018  

- Built a Python middle layer interfacing SQL databases with Elasticsearch; deployed and maintained reporting service on AWS Linux.

**Junior Business Analyst - *TBC Bank*** - *Tbilisi, Georgia* May 2017 – Feb 2018  

- Produced system documentation and process diagrams within a Scrum-based innovations team.

HONORS

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- Handshake AI Fellow, *Handshake MOVE Program* Aug 2025 – Present
- Travel grant to present at APS March Meeting, *Binghamton University* 2022, 2023
- Bronze Medal, International Physics Olympiad (Tallinn, Estonia) 2012