SABA KHARABADZE, PHD

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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

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

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

- 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

Founding Member, Data Science / ML - ***Keepers*** - **https://kprs.pro** - *Remote* — Dec 2024 – Present

- Build ETL pipelines to ingest exchange data into internal databases using Python, SQLAlchemy, and SQL; implement data validation and cleaning in pandas.
- Develop anomaly detection and trend prediction on financial time-series using XGBoost and feature engineering pipelines.
- Produce research analyses and monitoring reports to support strategy development and ongoing performance review.

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

- 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