SABA KHARABADZE, PHD

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Pisa, Tuscany, Italy

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.

Bachelor of Science in Physics
Free University of Tbilisi — May 2017
Minor in Computer Science and Mathematics

SKILLS

Technical Skills Machine learning, neural networks, Python (PyTorch, JAX, pandas, NumPy, SciPy), C/C++, git, Docker, GPU computing (CUDA, multi-GPU training), distributed training, HPC systems, Linux system administration, shell scripting, materials modeling: DFT (VASP, Gaussian), SQL

Languages English (native/bilingual), Russian (proficient), Georgian (native/bilingual)

ACADEMIC EXPERIENCE

Research Scientist ∘ ***CNIT RaSS Lab*** - *Pisa, Italy* — April 2025 - present

- Utilizing ML approach for radar signal processing and target detection.
- Building simulation frameworks for coverage analysis of mono- and multistatic radar systems.

Physics AI model validation expert ∘ ***Handshake MOVE Program*** - *Remote* — August 2025 - present

- Creating reasoning problems and solutions for AI models to challenge their physics knowledge.
- Evaluating AI model responses and providing feedback to improve their understanding of physics concepts.

PhD Candidate ∘ ***Binghamton University*** - *Binghamton, NY* — August 2018 - August 2024

- **Discovery of new Li-Sn phases with machine learning** — November 2020 - May 2022
  - Generated **DFT** reference data in-house using **VASP** software to parametrize a **neural network** model written in **C**, with a particular application on the Li-Sn system aligned with our research objectives.
  - Utilized **evolutionary algorithms** and **GPU-accelerated computing** to produce more than 1 million structures and 1 terabyte of energy-force data, leveraging HPC clusters for massively parallel simulations.
  - Developed **Python** pipelines for large-scale data processing and analysis of **numerical results** into **physical, electrochemical, and structural properties**.
  - Identified 8 new stable structures that redefined the previously known convex hulls for Li-Sn system for ambient and elevated pressures.
  - Conducted **phonon** calculations at ML and DFT levels to assess and confirm stability of newly discovered structures at elevated temperatures.
  - First authored and published the manuscript in Nature Partnered Journals Computational Materials under the title: "*Prediction of stable Li-Sn compounds: boosting ab initio searches with neural network potentials*".
- **Stability analysis of potentially superconducting LiBC compounds** — August 2022 - February 2023
  - Calculated Li chemical potential in Li_xBC to estimate conditions required for delithiation of LiBC parent material.
  - Examined B–C phases to explain metastable BC_3 polymorphs with honeycomb and diamond-like morphologies.
  - Employed evolutionary optimization and rational design to identify more natural and favorable Li_2B_2C configurations, still above thermodynamic stability threshold.

- Conducted **phonon** calculations in the quasi-harmonic approximation framework to gain further insight into stability at varying volumes and assess contribution of anharmonic effects.
- First authored and published the manuscript in Physical Chemistry Chemical Physics under the title: "*Thermodynamic stability of Li–B–C compounds from first principles*".

- **Implementation of *NPT* barostat molecular dynamics module** January 2020 - May 2020
  - Implemented *NPT* barostat in **C** for **molecular dynamics** package which is now a part of group's in-house atomic simulation software MAISE (available at https://github.com/maise-guide/maise).
  - Tested the module and obtained thermal expansion coefficients for silver, copper, and sodium that were within 10% of experimental values.
  - Coauthored the resulting paper where I wrote the section regarding molecular dynamics. Paper was published in Computer Physics Communications under the title: "*MAISE: Construction of neural network interatomic models and evolutionary structure optimization"*.
- **Development of documentation website for group's software MAISE** May 2020 - August 2020
  - Developed wiki in **Python** using Sphinx library that is now hosted on https://maise.binghamton.edu/wiki/.
  - Wrote the section about **molecular dynamics**.
- **Working as a university computational system administrator** August 2020 - May 2021
  - Administered two university-wide **HPC Linux** computing clusters each with over 1,000 cores and **GPU nodes**.
  - Installed and maintained various computational software including **Intel** and **GNU** compilers, **Python**, **PyTorch**, **NumPy**, **SciPy**, **Jupyter**, **OpenMPI**, **CUDA toolkit**, **VASP**, **ORCA** and others. Set each software up for parallel multi-node and multi-GPU use.
  - Configured job scheduling systems and resource allocation for distributed computing workloads.

PUBLICATIONS

"Thorn, A., Gochitashvili, D., **Kharabadze, S.**, Kolmogorov, A.N. (2023) Machine learning search for stable binary Sn alloys with Na, Ca, Cu, Pd, and Ag. Phys. Chem. Chem. Phys., 2023, 25, 22415-22436."

"**Kharabadze, S.**, Meyers, M., Tomassetti, C. R., Margine, E. A., Mazin, I. I., Kolmogorov, A.N. (2023) Thermodynamic stability of Li-B-C compounds from first principles. Phys. Chem. Chem. Phys., 2023, 25, 7344-7353."

"**Kharabadze, S.**, Thorn, A., Koulakova, E.A., Kolmogorov, A. N. (2022) Prediction of stable Li-Sn compounds: boosting ab initio searches with neural network potentials. npj Comput Mater 8, 136."

"Singh, J., Behatha, A., **Kharabadze, S.**, Kolmogorov, A. N., Vaitheeswaran, G., & Kanchana, V. (2022). Prediction of Ground State Structures and Robust Weyl Fermionic States in MnRhP. The Journal of Physical Chemistry C. 126, 40, 17328-17337"

"Hajinazar, S., Thorn, A., Sandoval, E. D., **Kharabadze, S.**, Kolmogorov, A. N. (2021). MAISE: Construction of neural network interatomic models and evolutionary structure optimization. Computer Physics Communications, 259, 107679."

PRESENTATIONS

"Kharabadze S. (2024). Machine Learning and ab initio insights into the design of lithium-based materials. Public thesis defense, Binghamton University. Committee: Dr. Alexey Kolmogorov, Dr. Wei-Cheng Lee, Dr. Bruce White, Dr. Mengen Wang. May 1st, 2024"

"Kharabadze S, Meyers M, Tomassetti C, Margine E, Mazin I, Kolmogorov A. (2023). Ab initio analysis of Li-B-C structure stability. In APS March Meeting Abstracts 2023 (Vol. 2023, pp. Q28-008)."

"Kharabadze, S., Thorn, A., Sandoval, E., Hajinazar, S., & Kolmogorov, A. (2022). Development of neural network interatomic potentials for accelerated prediction of stable compounds. In APS March Meeting Abstracts (Vol. 2022, pp. F47-007)."

"Kharabadze S. (2021). Use of Machine Learning methodology in materials discovery. International Society of Georgian Scientists, STEM symposium, October 2021"

"Kharabadze S. (2021). Materials design with machine learning and ab initio methods. Preliminary thesis defense, Binghamton University. Committee: Dr. Alexey Kolmogorov, Dr. Manuel Smeu, Dr. Bruce White"

PROFESSIONAL EXPERIENCE

Back-end Developer ∘ ***Eleven Wireless*** - *Portland, OR (remote)* October 2017 - April 2018

- Developed a **Python** middle layer interfacing **SQL** databases and **ElasticSearch** engine.
- Deployed and maintained ticket reporting project on **AWS** Linux instance. The reporting portal was constantly online with live patching.

Junior Business Analyst ∘ ***TBC Bank*** - *Tbilisi, Georgia* May 2017 - February 2018

- Constructed flow diagrams for ATMs while working in an innovations team.
- Wrote system documentation for software engineering side while working within Scrum framework.

Software Engineer Intern ∘ ***Bank of Georgia*** - *Tbilisi, Georgia* May 2016 - December 2016

- Learned the software development foundations of the bank, got acquainted with the day-to-day process of problem setting and implementation.

TEACHING EXPERIENCE

Teaching assistant in general physics ∘ ***Binghamton University*** - *Binghamton, NY* August 2018 - August 2020

- Taught intro physics as a TA and achieved 85% positive feedback with 67% participation.
- Instructed new TAs as a head teaching assistant during the second year.

Coach of physics team ∘ ***42nd School of physics and mathematics*** - *Tbilisi, Georgia* September 2012 - May 2018

- Coached a class of high school students for physics competitions. Students got awarded multiple medals in local and international competitions.
- Lead the school team of 11 students at the 2016 International Zhautykov Olympiad in Almaty, Kazakhstan. Our team got awarded with silver medal in physics and mathematics.

HONORS AND AWARDS

- Handshake AI Fellow, *Handshake MOVE Program* August 2025 - present
- Travel grant to present at APS March meeting, *SUNY Binghamton University* March 2022, 2023
- Merit-based tuition scholarship, *Free University of Tbilisi* August 2012
- Bronze medal, *43rd International Physics Olympiad (Tallinn, Estonia)* July 2012
- Bronze medal in physics, *8th International Zhautykov Olympiad (Almaty, Kazakhstan)* January 2012
- Honorable mention, *42nd International Physics Olympiad (Bangkok, Thailand)* July 2011
- 1st place in national physics olympiad, *Tbilisi, Georgia* May 2007, 2008, 2010