Tara Karimzadeh Sabet

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Summary

Ambitious computational materials scientist with expertise in high-performance computing, first-principles calculations, and machine learning. Adept at thriving in multidisciplinary teams and independent research settings. Excellent interpersonal, problem-solving, and presentation skills, with a proven ability to communicate complex findings to diverse audiences through teaching and presentations. Demonstrated agility in mastering new skills and a strong commitment to driving innovation in sustainable energy and thermal management technologies.

Education

Doctor of Philosophy in Materials Science *Expected May 2027*

Carnegie Mellon University *Pittsburgh, PA*

- **Thesis Advisor:** Dr. Ismaila Dabo
- **Thesis:** First Principles Study of Vibrational Modes and Heat Transport in High-Entropy Oxides

Master of Science in Materials Science and Engineering *Jan 2025 – Dec 2025*

Carnegie Mellon University *Pittsburgh, PA*

- **Selected Coursework:** Introduction to Machine Learning, Methods of Computational Materials Science, Quantum Chemistry (I & II)

Bachelor of Science in Materials Engineering | Concentration: Materials Design *Aug 2016 – Aug 2020*

Iran University of Science and Technology *Tehran, Iran*

- **Thesis:** Solution Combustion Synthesis of Iron Oxide Nanoparticles for Supercapacitors
- **Selected Coursework:** Design & Selection of Engineering Materials, Thermodynamics of Materials, Economics & Industrial Management

Work Experience

Teaching Assistant *Jan 2025 – Dec 2025*

Department of Materials Science and Engineering, Carnegie Mellon University *Pittsburgh, PA*

- *Methods of Computational Materials Science* (Spring 2025) and *Foundations of Materials Science and Engineering* (Fall 2025).
- Designed and led engaging, hands-on recitation sessions building on core concepts and problem-solving across multiple topics.
- Assisted instructors with course development and preparation, including lectures, homework problems, solutions, and recitation materials.
- Held open office hours to support students with coursework, assignments, and coding/software exercises.
- Graded exams, quizzes, and homework/laboratory assignments, ensuring timely and detailed feedback.

Research Assistant *Jan 2025 – Present*

Department of Materials Science and Engineering, Carnegie Mellon University *Pittsburgh, PA*

- Established a materials design framework for thermoelectrics by leveraging ab initio phonon calculations and Debye-based thermal conductivity modeling to predict transport properties in complex oxides.
- Evaluated ballistic and hydrodynamic formulations of the Boltzmann transport equation against atomistic calculations to address nanoscale heat transport predictions, providing a framework for optimal thermal management in quantum and semiconductor devices.
- Leveraged machine learning interatomic potentials to accelerate the prediction of vibrational modes and heat transport in high-entropy oxides.
- Co-authored peer-reviewed research and perspective papers in top-tier journals, utilizing computational modeling insights to advance the field of thermal management and thermoelectrics.

Teaching Assistant *Sep 2022 – May 2024*

Department of Materials Science and Engineering, Pennsylvania State University *University Park, PA*

- *Thermodynamics of Materials* (Fall 2022) and *Computational Materials Science* (Spring 2023 & Spring 2024).
- Conducted recitations and office hours to support student learning and problem-solving.
- Evaluated homework, laboratory assignments, and exams, providing detailed feedback to reinforce key concepts.

Research Assistant *Aug 2021 – Present*

Center for Nanoscale Science, Materials Research Science & Engineering Center (MRSEC) *University Park, PA*

- Studied structure–property relationships in high-entropy metal oxides via high-performance computing and first-principles calculations to evaluate compositional stability, electric polarization and thermal properties for electrocaloric and thermoelectric energy conversion systems.
- Spearheaded the computational arm of multiple NSF-funded cross-disciplinary projects, collaborating closely with experimental teams to advance energy research.
- Directed weekly interdisciplinary research meetings, managing presentation schedules and maintaining comprehensive documentation to support ongoing project collaboration.

Summer Research Intern *Jul 2019 – Sep 2019*

Iran Khodro Automotive Company *Tehran, Iran*

- Conducted mechanical and quality tests on auto bodies and coatings in R&D lab via cross-cut, stone chip, gas chromatography, and colorimetry.
- Crafted a comprehensive handbook on pretreatment/electrodeposition processes, detailing chemical reactions and operational procedures.
- Compared spray versus immersion phosphating on auto body panels through mechanical testing, demonstrating superiority of immersion.

Skills

Materials Science	Quantum ESPRESSO, VASP, Phonopy/Phono3py, CrystalMaker, Ovito, VESTA, ASE, ICET, Pymatgen, FactSage
Programming & Scripting	Python (Pandas, NumPy, SciPy, Scikit-learn, Matplotlib, Seaborn, Plotly), C/C++, Bash, C#, MATLAB, HTML
Software & Development	Git/GitHub, Docker, Linux OS, Jupyter, Visual Studio, PyCharm, LaTeX
Machine Learning	Deep Learning, Neural Networks, Random Forests, Bayesian Optimization, Generative AI, LLMs, MLIPs
Cloud & HPC	AWS (SageMaker), Linux OS, Docker, Slurm/PBS Schedulers, GPU Acceleration (CUDA), Parallelization (MPI)
General/Engineering	SolidWorks, ANSYS Mechanical, ANSYS Granta Selector, Origin, Microsoft Office Suite (Proficient)
Languages	Persian (Native Speaker), English (Fluent), French (Intermediate), German (Intermediate), Dutch (Intermediate)

Additional Training

Improving Deep Neural Networks *Feb 2025*

DeepLearning.AI *Credential ID: BXIKJSH2IY7J*

- Leveraged systematic approaches to improve deep neural networks, including hyperparameter tuning, bias/variance analysis, regularization (L2, dropout), optimization algorithms (Momentum, RMSprop, Adam), batch normalization, and implementation in TensorFlow.

Generative AI with Large Language Models *Sep 2024*

DeepLearning.AI *Credential ID: HVN9VG3I5ZK1*

- Gained in-depth understanding of the transformer architecture, LLM training, fine-tuning, scaling laws, model evaluation, optimization, and real-world deployment strategies using Python and AWS SageMaker.

Neural Networks and Deep Learning *Sep 2024*

DeepLearning.AI *Credential ID: Z2GI1J9WJTBK*

- Built foundational expertise in deep learning by implementing neural networks from scratch, including forward/backpropagation, vectorization, shallow and deep architectures, and practical application of CNNs and RNNs using Python.

Achievements

2026 **Recipient of the MSE Teaching Intern Award**, Carnegie Mellon University *Pittsburgh, PA*

2025 **Recognized by Students through *Thank a Teacher* for Impactful Teaching**, Carnegie Mellon University *Pittsburgh, PA*

2023 **Recipient of the Materials Science and Engineering Travel Award**, Pennsylvania State University *University Park, PA*

2020 **Merit-Based Exemption from the Graduate Entrance Exam**, Iran University of Science & Technology *Tehran, Iran*

2020 **Top-Ranked Student in the 2020 Engineering Materials Design Cohort**, Iran University of Science and Technology *Tehran, Iran*

2019 **Recipient of the Academically Outstanding Student Award**, Iran University of Science & Technology *Tehran, Iran*

2015 **1st and 2nd Phase Qualifier in the National Physics Olympiad**, Iran Physics Olympiad *Tehran, Iran*

2014 **Earned Selection Among Top Team Projects to Present at 21st iEARN Global Conference**, International Education and Resource Network (iEARN) *Tehran, Iran*

2012 **Admitted into elite specialized schools for gifted students via a highly competitive nationwide entrance exam testing the top percent of students**, National Organization for the Development of Exceptional Talents *Tehran, Iran*

Presentations & Publications

Publications

[1] *Nanoscale Confinement of Phonon Flow and Heat Transport*. A. Beardo, W. Chen, B. McBennett, T. Karimzadeh Sabet, E. Nelson, T. Culman, H. Kapteyn, J. Knobloch, M. Murnane, I. Dabo. *npj Computational Materials*, 11 (1), p. 172, 2025. doi: https://doi.org/10.1038/s41524-025-01593-7.

[2] *High-Entropy Design of Transition Metal Oxide Semiconductors with Ultra-Low Thermal Conductivity*. R. Robinson, T. Karimzadeh Sabet, F. Marques dos Santos Vieira, S. S. I. Almishal, S. V. G. Ayyagari, R. Katzbaer, G. Di Gianluca, S. Sarker, P. R. Trinidad-Perez, J. P. Barber, S. Gelin, S. H. Lee, J. Hodges, R. E. Schaak, V. H. Crespi, V. Gopalan, N. Alem, C. M. Rost, J-P. Maria, I. Dabo, Z. Mao. *Communications Materials*, 2026. doi: https://doi.org/10.1038/s43246-026-01103-2.

Conference Presentations

[1] *Ultra-low heat conductivity by configurational entropy for thermoelectric conversion*. T. Karimzadeh Sabet. *American Physical Society Global Physics Summit*, Anaheim (CA), March 2025. **Oral Presentation**.

[2] *Electrocaloric performance of high-entropy oxides from first principles*. T. Karimzadeh Sabet. *Materials Research Society Spring Meeting & Exhibit*, Seattle (WA), April 2024. **Invited Talk**.

[3] *Electrocaloric performance of high-entropy perovskites from first principles*. T. Karimzadeh Sabet. *American Physical Society March Meeting*, Minneapolis (MN), March 2024. **Oral Presentation**.

[4] *Electric polarization in high-entropy oxides for electrocaloric refrigeration*. T. Karimzadeh Sabet. *American Physical Society March Meeting*, Las Vegas (NV), March 2023. **Poster Presentation**.

[5] *First-principles prediction of the phase stability of high-entropy oxides*. T. Karimzadeh Sabet. *American Physical Society March Meeting*, Las Vegas (NV), March 2023. **Oral Presentation**.

[6] *Temperature-dependent compositional stability and electric polarization of high-entropy oxides in electrocaloric cooling applications*. T. Karimzadeh Sabet. *Conference Across MRSEC-PREM Schools*, Columbus (OH), November 2022. **Poster Presentation**.

Leadership & Service

Vice President
Apr 2024 – Dec 2024

Multicultural Engineering Graduate Association *University Park, PA*

- Spearheaded "MEGA Works," a series of structured academic co-working sessions to provide STEM graduate students with a productive, well-resourced environment—complete with amenities—focused on peer accountability and work progress.
- Co-organized events and professional development workshops, managing end-to-end logistics to maximize attendance and engagement.
- Co-launched the Graduate Student Community Space, to establish a multi-functional campus hub for studying, networking, and socialization.

Secretary
Apr 2023 – Apr 2024

Multicultural Engineering Graduate Association *University Park, PA*

- Facilitated executive board meetings to strategize, design, and execute technical/professional development workshops and networking events.
- Centralized organizational workflows by maintaining detailed records of meeting logs, logistics, event metrics, and actionable milestones.

Career Fair Exhibitor
Nov 2023

Center for Engineering Outreach and Inclusion, Penn State College of Engineering *Salt Lake City, UT*

- Represented Penn State Graduate School's College of Engineering as a graduate track sponsor and promoted recruitment opportunities at the Society of Hispanic Professional Engineers (SHPE) National Convention in Salt Lake City.
- Served as an ambassador at the Advanced Degree Showcase, actively engaging with prospective applicants to promote graduate programs.

Workshop Facilitator
Jul 2022 – Feb 2024

Penn State Eberly College of Science *University Park, PA*

- Designed activities and educated K-12 students on sustainability and materials science through MRSEC outreach activities, such as the life cycle analysis of cell phones on the costs and carbon emissions—from extracting raw materials to production and shipping.
- Facilitated the following workshops: Science-U (Make it Matter) July 2022 & 2023, Exploration-U (Bellefonte Family STEAM Night) November 2023, ENVISION (STEM Career Day Supporting Young Women) February 2023 & 2024.

Volunteer of the Youth Project
Nov 2013 – Jul 2014

International Education and Resource Network *Tehran, Iran*

- Spearheaded efforts in a high-impact team project that earned recognition and selection from a competitive pool of participating groups to be showcased at the 21st iEARN International Conference in Buenos Aires, Argentina.
- Managed community outreach and global communications for the "Volunteer of Youth" initiative; coordinated fundraising initiatives for pediatric cancer patients as well as volunteer operations at nursing homes, orphanages, and specialized care facilities.