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 research.

Education

Doctor of Philosophy in Materials Science *Expected Dec 2026*

Carnegie Mellon University *Pittsburgh, PA*

- **Thesis Advisor:** Dr. Ismaila Dabo
- **Thesis:** First-principles study of phonon transport in high-entropy oxides for thermoelectric applications

Master of Science in Materials Science and Engineering *Aug 2021 – 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 *Aug 2016 – Aug 2020*

Iran University of Science and Technology *Tehran, Iran*

- **Thesis:** Solution combustion synthesis of iron oxide nanoparticles for supercapacitors

Work Experience

Teaching Assistant | Foundations of Materials Science and Engineering *Aug 2025 - Dec 2025*

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

- Designed and led engaging, hands-on recitation sessions building on the concepts and problem-solving for various topics in Materials Science.
- Actively helped instructors with course design and materials preparation (lectures, homework problems, solutions, recitations).
- Conducted open office hours to assist with coursework, assignments and coding/software exercises.
- Graded course deliverables, e.g., exams, quizzes, and homework assignments.

Teaching Assistant | Methods of Computational Materials Science *Jan 2025 - May 2025*

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

- Instructed students on topics including Molecular Dynamics, Electronic-Structure Methods, Phase-Field Models, and Machine Learning.
- Led hands-on recitations to aid with homework assignments and coding/software exercises.
- Graded course deliverables, e.g., homework and laboratory assignments, and managed a virtual Piazza platform to facilitate communication.

Research Assistant *Jan 2025 - Present*

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

- Explored vibrational properties and thermal transport in complex oxides for sustainable energy applications via ab initio phonon calculations.
- Leveraged GNN-based machine learning interatomic potentials (MLIPs) to accelerate the prediction of vibrational modes via transfer learning.

Teaching Assistant | Computational Materials Science *Jan 2023 - May 2024*

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

- Conducted recitations and office hours to assist with course materials and address learning needs effectively.
- Evaluated homework and laboratory assignments, providing detailed individual feedback to reinforce key concepts.

Teaching Assistant | Thermodynamics of Materials *Sep 2022 - Dec 2022*

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

- Held recitations to assist with homework assignments for a graduate core course.
- Proctored exams and graded course deliverables.

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 crystalline oxides via first-principles methods for electrocalorics and thermoelectrics.
- Managed weekly meetings across IRG-2, organized presentation schedules, and maintained detailed meeting records.

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.

Research Projects

Hybrid ML-DFT approach for thermal properties and vibroscopic analysis *Jan 2025 - Present*

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

- Studied phonon band unfolding and non-analytical corrections in complex oxides to facilitate vibrational property predictions.
- Performed virtual crystal approximation (VCA) to improve the prediction of phonon properties in disordered structures.
- Worked on improving machine learning interatomic potentials (MLIPs) in phonon calculations via Bayesian optimization and transfer learning.

Infrared and Raman spectra of III-V semiconductors *May 2024 - Present*

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

- Implemented density functional perturbation theory to calculate phonon dispersion relations and vibrational density of states.
- Supplemented information on vibrational modes by computing the infrared and Raman spectra via first principles.

Thermal conductivity of high-entropy wolframites *Jan 2024 - Present*

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

- Performed phonon calculations via finite displacements and supercell approaches to obtain harmonic/anharmonic interatomic force constants.
- Coded a mathematical workflow to model thermal conductivity using theoretically calculated vibrational properties.
- Extracted various phonon scattering contributions to an ultra-low thermal conductivity in the high-entropy phase.
- Designed a highly-efficient Bash/Python workflow for managing calculation jobs to optimize computational resource allocation.

Electrocaloric properties of high-entropy oxides via first principles *Aug 2021 - Dec 2023*

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

- Analyzed compositional stability of A- and B-site disorder in high-entropy perovskites via first principles.
- Visualized the effects of short-range ordering on the energetics of perovskites using an elastic polyhedra model and strain ellipsoids.
- Developed a model using energy landscapes to interpret temperature-dependent polarization and electrocaloric properties of ferroelectrics.

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)

Achievements

2025	**Recognized by students through *Thank a Teacher* for impactful teaching**, Carnegie Mellon University	*Pittsburgh, PA*
2023	**Recipient of the DMSE Travel Award**, Penn State Department of Materials Science and Engineering	*University Park, PA*
2020	**Merit-Based Exemption from the Graduate Entrance Exam**, Iran University of Science & Technology	*Tehran, Iran*
2020	**Top-Ranked Student in Engineering Materials Design Cohort**, Iran University of Science and Technology	*Tehran, Iran*
2019	**Academically Outstanding Student Award**, Office of Talent, Iran University of Science & Technology	*Tehran, Iran*
2015	**1st and 2nd Phase Qualifier in the National Physics Olympiad**, Iran Physics Olympiad	*Tehran, Iran*
2014	**Showcased Project at 21st iEARN Conference**, International Education and Resource Network	*Tehran, Iran*
2012	**Admitted to School for Gifted Students**, National Organization for the Development of Exceptional Talents	*Tehran, Iran*

Presentations & Publications

Conference Presentations

"Ultra-low heat conductivity by configurational entropy for thermoelectric conversion", APS Global Physics Summit, Anaheim, CA, 18 March 2025. **Oral Presentation**.

"Electrocaloric performance of high-entropy oxides from first principles", Materials Research Society Spring Meeting & Exhibit, Seattle, WA, 24 April 2024. **Invited Talk**.

"Electrocaloric performance of high-entropy perovskites from first principles", American Physical Society March Meeting, Minneapolis, MN. 4 March 2024. **Oral Presentation**.

"Electric polarization in high-entropy oxides for electrocaloric refrigeration", American Physical Society March Meeting, Las Vegas, NV. 9 March 2023. **Poster Presentation**.

"First-principles prediction of the phase stability of high-entropy oxides", American Physical Society March Meeting, Las Vegas, NV. 8 March 2023. **Oral Presentation**.

"Temperature-dependent compositional stability and electric polarization of high-entropy oxides in electrocaloric cooling applications", Conference Across MRSEC-PREM Schools, Columbus, OH. 9 November 2022. **Poster Presentation**.

Publications

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** (172). 2025

High-Entropy Design of Transition Metal Oxide Semiconductors with Ultra-Low Thermal Conductivity
R. A. 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

Leadership & Service

Vice President *University Park, PA*

Multicultural Engineering Graduate Association *Apr 2023 – Present*

- Spearheaded MEGA Works, aimed at providing a collaborative working/writing space for graduate students to built support and accountability.
- Co-organized events and workshops, and managed logistics to boost attendance and engagement.
- Helped launch the Graduate Community Space, a dedicated lounge fostering collaboration, study sessions, and events for STEM students.

Secretary *University Park, PA*

Multicultural Engineering Graduate Association *Apr 2023 – Present*

- Facilitated executive board meetings to plan technical and professional development workshops as well as social networking events.
- Maintained a detailed record of executive board meeting notes, past/upcoming events, planning logistics, and actions items.

Career Fair Exhibitor, Society of Hispanic Professional Engineers National Convention *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.
- Actively engaged with attendees at the Advanced Degree Showcase for graduate school recruitment.

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 Volunteer of Youth group project that earned recognition and was selected from a competitive pool of groups participating in the iEARN program to be showcased at the 21st iEARN International Conference in Buenos Aires, Argentina.
- Managed communications and coordinated fundraising initiatives for children battling cancer as well as volunteer efforts at nursing homes.