

# 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

Carnegie Mellon University

Expected Dec 2026

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

Carnegie Mellon University

Aug 2021 – Dec 2025

Pittsburgh, PA

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

### Bachelor of Science in Materials Engineering

Iran University of Science and Technology

Aug 2016 – Aug 2020

Tehran, Iran

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

## Work Experience

### Teaching Assistant | Foundations of Materials Science and Engineering

Department of Materials Science and Engineering, Carnegie Mellon University

Aug 2025 - Dec 2025

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

Department of Materials Science and Engineering, Carnegie Mellon University

Jan 2025 - May 2025

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 laboratory exercises.
- Graded course deliverables, e.g., homework and laboratory assignments, and managed a virtual Piazza platform to facilitate communication.

### Research Assistant

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

Jan 2025 - Present

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

Department of Materials Science and Engineering, Pennsylvania State University

Jan 2023 - May 2024

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

Department of Materials Science and Engineering, Pennsylvania State University

Sep 2022 - Dec 2022

University Park, PA

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

### Research Assistant

Center for Nanoscale Science, Materials Research Science & Engineering Center (MRSEC)

Aug 2021 - Present

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

Iran Khodro Automotive Company

Jul 2019 - Sep 2019

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 based on Debye, Klemens, and Callaway contributions 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

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

# Achievements

2023	<b>Recipient of the DMSE Travel Award</b> , Penn State Department of Materials Science and Engineering	University Park, PA
2020	<b>Merit-Based Exemption from the Graduate Entrance Exam</b> , Iran University of Science & Technology	Tehran, Iran
2020	<b>Top-Ranked Student in Engineering Materials Design Cohort</b> , Iran University of Science and Technology	Tehran, Iran
2019	<b>Academically Outstanding Student Award</b> , Office of Talent, Iran University of Science & Technology	Tehran, Iran
2015	<b>1st and 2nd Phase Qualifier in the National Physics Olympiad</b> , Iran Physics Olympiad	Tehran, Iran
2014	<b>Showcased Project at 21st iEARN Conference</b> , International Education and Resource Network	Tehran, Iran
2012	<b>Admitted to School for Gifted Students</b> , 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. McBenett, T. Karimzadeh Sabet, E. Nelson, T. Culman, H. Kapteyn, J. Knobloch, M. Murnane, I. Dabo  
*npj Computational Materials* p. 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* (under revision). 2025

### Probing Vibrational Modes in High-Entropy Rock Salt Structures

T. Karimzadeh Sabet, S. V. G. Ayyagari, S. Gelin, N. Alem, I. Dabo  
(in preparation). 2026

## Leadership & Service

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### 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.
- Actively helped with event and workshop planning, .

### 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.

### Graduate School Career Fair Exhibitor, Society of Hispanic Professional Engineers (SHPE)

Nov 2023

#### Center for Engineering Outreach and Inclusion, Penn State College of Engineering

Salt Lake City, UT

- Represented Penn State's Graduate School/College of Engineering as a graduate track sponsor and promoted recruitment opportunities at SHPE's National Convention.
- 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 from the costs and carbon emissions of 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.