

Vahe Gharakhanyan

New York, NY

☎ (510) 333-6330 | ✉ vg2471@columbia.edu | 🏠 gvahe.github.io | 🌐 gvahe | in vahegharakhanyan

Education

Columbia University

Aug 2019 - present

PHD MATERIALS SCIENCE AND ENGINEERING

GPA: 4.33 / 4.00

MS MATERIALS SCIENCE AND ENGINEERING

GPA: 4.04 / 4.00

- Relevant Coursework: Machine Learning, Computational Math, Numerical Methods, Atomistic Simulations, Computing Electronic Structure, Phonon Calculations, Electric, Magnetic and Mechanical Properties, Crystallography.

University of California, Berkeley

Aug 2015 - May 2019

BS MATERIALS SCIENCE AND ENGINEERING, BS CHEMICAL ENGINEERING

GPA: 3.61 / 4.00

MINOR ELECTRICAL ENGINEERING AND COMPUTER SCIENCES

- Relevant Coursework: Optical Engineering, Integrated Circuit Design, Information Systems, Dynamics and Control, Polymeric Materials, Thin Films, Materials Production and Design, Mass and Energy Transport, Fluid Dynamics, Phase Transformations and Kinetics, Reactor Engineering, Crystal Defects, Corrosion, Quantum Mechanics, Data Science, Data Structures, Discrete Math and Probability.
- **Coursework in Pharmaceutical sciences:** Molecular Biology, Microbiology, Genetics, Org. Biochem. 2013 - 2015

Work Experience

Google X (X - The Moonshot Factory)

Jun 2022 - present

AI RESIDENT (GENERATIVE MODELS FOR MATERIALS DISCOVERY, COMPUTER VISION)

Mountain View, CA

- X is Alphabet's moonshot factory. I am part of a confidential team, working in the area of ML for materials recycling.
- Co-developed a patent and a workshop paper (see below) for applications related to materials discovery.

Google X (X - The Moonshot Factory)

May 2021 - Dec 2021

AI RESIDENT (GENERATIVE MODELS FOR MOLECULAR DISCOVERY)

Mountain View, CA

- Co-developed four patents (see below) for applications related to molecular discovery.

The Quant Edge

Aug 2020 - Feb 2021

QUANTITATIVE RESEARCH INTERN (ML TRACK)

New York, NY

- Worked towards predicting soccer match results using a team-strength metric and a Poisson model for scoring, and simulating overall league standings using Monte Carlo method.
- Developed a ranking algorithm for predicting horse racing results from pairwise scores.

Research Experience

Urban Group at Columbia University

Oct 2019 - present

ML & QUANTUM-GUIDED INVERSE DESIGN OF MATERIALS WITH TARGET PROPERTIES

New York, NY

- Employing (modifications of) variational autoencoders (VAEs) for inverse design of materials with desired properties.
- Representation learning of structures from local atomic environments and compression with information theory.
- Learning materials (alchemical) similarity metric from the latent space to be used in ML force-fields (ML-FF).
- Used symbolic regression to understand different melting and free energy behaviors within clusters of materials.
- Worked towards learning about different forms of melting from combined ML, short-time MD and DFT computations.

Asta Group at UC Berkeley

Mar 2018 - May 2019

THERMODYNAMICS OF CHARGED DEFECTS WITH DENSITY FUNCTIONAL THEORY

Berkeley, CA

- Employed DFT to understand how the surrounding of each atom changes after charged defect incorporation in TiO_2 .
- Used Python Charged Defect Toolkit (PyCDT) to post-process charged defect calculations.

Papers

- Garrido Torres, J. A., **Gharakhanyan, V.**, Artrith, N., Eegholm, T. H., and Urban, A. (2021). Augmenting zero-Kelvin quantum mechanics with machine learning for the prediction of chemical reactions at high temperatures. *Nature communications*, 12(1), 1-9. (doi:10.1038/s41467-021-27154-2)
- Gadhiya, T., Shah, F., Vyas, N., **Gharakhanyan, V.**, Yang, J. H., and Holiday, A. (2022). Directional Variational Transformers for continuous molecular embedding. *ELLIS 2022 ML4Molecules workshop*. (jku.at)
- **Gharakhanyan, V.**, Aalto, M. S., Alsoulah, A., Artrith N., and Urban, A. (2023). Constructing and compressing global moment descriptors from local atomic environments. (2023). *ICLR 2023 ML4Materials workshop*.

- **Gharakhanyan, V.**, Wirth, L., Garrido Torres, J. A., Eisenberg, E., and Urban, A. (2023). Discovering melting-temperature prediction models of inorganic solids by combined regression and clustering. [in preparation]
- **Gharakhanyan, V.**, Wang, T., Chatterjee, S., Trinkle, D. R., and Urban, A. (2023). ML-accelerated molecular dynamics simulations for predicting equilibrium melting points from short non-equilibrium simulations. [in preparation]
- **Gharakhanyan, V.**,[†] Aalto, M. S.,[†] and Urban, A. (2023). Measuring the transferability of materials embeddings. ([†] equal contribution) [in preparation]
- Wirth, L., **Gharakhanyan, V.**, Thompson, M., Lu, Z., Wang, T., Gonzalez, D., Chatterjee, S., Urban, A. and Trinkle, D. R. (2023). Representation of free energy surfaces of binary alloy systems from CALPHAD through symbolic learning studies. [in preparation]

Patents

- **Gharakhanyan, V.**, Yang, J. H., Gadhiya, T., Holiday, A. (2022). Search for candidate molecules using quantum or thermodynamical simulations and autoencoder. *U.S. Patent App.*, filing date Oct 17, 2022.
- Yang, J. H., **Gharakhanyan, V.**, Gadhiya, T., Holiday, A. (2022). Ionic liquid-based depolymerization optimization. *U.S. Patent App.*, filing date Oct 17, 2022.
- Holiday, A., Gadhiya, T., **Gharakhanyan, V.**, Yang, J. H., Vyas, N., Shah, F. (2022). Depolymerization optimization platform. *U.S. Patent App.*, filing date Oct 17, 2022.
- Gadhiya, T., Holiday, A., Shah, F., Vyas, N., Yang, J. H., **Gharakhanyan, V.** (2022). Molecular structure transformers for property prediction. *U.S. Patent App.*, filing date Oct 17, 2022.
- Holiday, A., **Gharakhanyan, V.**, Gadhiya, T., Vyas, N., and Shah, F. (2023). Machine learning platform for finding solid catalysts for depolymerization reactions. *U.S. Provisional Patent App.*, filing date Feb 8, 2023.

Presentations and Posters([†])

- Navigating materials design space with autoencoders to learn materials thermodynamics. APS March Meeting, March 2023, Las Vegas, NV.
- Machine learning and quantum-guided modeling of metal oxide thermodynamic properties. APS March Meeting, March 2023, Las Vegas, NV. ([†])
- Combined clustering and regression for predicting melting temperatures of solids. 2022 TMS Annual Meeting, March 2022, Anaheim, CA.
- Machine learning and quantum-guided modeling of metal oxide thermodynamic properties. AIChE 4th Battery and Energy Storage Conference, The City College of New York, October 2022, New York, NY. ([†])
- Machine learning and quantum-guided modeling of metal oxide thermodynamic properties at high temperatures. Columbia Electrochemical Energy Center Symposium, Columbia University, September 2022, New York, NY. ([†])
- Thermodynamics of redox reactions at high temperatures with combined machine learning and density functional theory. Artificial Intelligence for Materials Science (AIMS) Workshop, July 2022, Virtual. ([†])
- Predicting melting temperatures of solids with combined clustering and regression. Artificial Intelligence for Materials Science (AIMS) Workshop, July 2022, Virtual. ([†])
- High-temperature chemical reactions with ML-augmented first-principles computations. Columbia University, Data Science Day, April 2022, New York, NY. ([†])
- Learning melting temperatures of binary materials with clustering and regression. Columbia University, Data Science Day, April 2022, New York, NY. ([†])

Awards

IMPACT Award for Excellence in Graduate Research by Data Science Group

Distinguished Student Award by Forum on International Physics

Mar 2023

GERA Energy Workshop Award and DMP Ovshinsky Student Prize

AMERICAN PHYSICAL SOCIETY

NSF Conference Fellowship

Jul 2021

MECHANISTIC ML AND DIGITAL TWINS (MMLDT-CSET) 2021 CONFERENCE

Data Science/Medical Research Program Fellowship

Jul 2020

TECHFOUNDATION, HARVARD MEDICAL SCHOOL

President's Special Award - Paper on Mathematical Modelling of Viruses PRESIDENT OF THE REPUBLIC OF ARMENIA - ARMEN SARKISSIAN [<i>press</i>]	<i>Jun 2020</i>
2nd place - Design Competition: The Energy Transition Challenge CHEVRON CORPORATION AND UC BERKELEY	<i>May 2018</i>
• Designed solar energy implementation into oil and gas company portfolios and inspired the global energy transition.	
Outstanding Tutor Award COLLEGE OF CHEMISTRY AT UC BERKELEY	<i>Dec 2017</i>
President's Annual Award for the Best Student in Information Technology SYNOPSIS, ARMENIA	<i>Oct 2013</i>
Two Bronze medals - International Chemistry Olympiads 2012 and 2013 WASHINGTON DC, USA AND MOSCOW, RUSSIA	<i>Jul 2012, Jul 2013</i>

Professional Service

Research Mentor - 2 Masters, 2 Undergraduate and 2 High-school students	<i>2020 - Present</i>
Reviewer - AI4Mat workshop @ NeurIPS, Journal of Chemical Physics	<i>2022 - Present</i>
Treasurer - Columbia Materials Advantage Student Chapter	<i>2021 - 2022</i>
Scholarship Reviewer - UC Berkeley Achievement Award Program	<i>May 2020</i>
Scholarship Reviewer - UC Berkeley Leadership Award Program	<i>May 2020</i>
Jury Member - Baltic Chemistry Olympiad	<i>2019 - 2020</i>
Team Member - Chemical Engineering Jeopardy, AIChE, UC Berkeley	<i>2017 - 2019</i>
Volunteer - Wikimedia Armenia	<i>2013 - 2015</i>

Teaching Experience

TA - Analysis of Engineering Problems course (CHEN 3020)	<i>Spring 2023</i>
TA - Atomistic Simulations course (CHEN 4880)	<i>Spring 2021</i>
TA - Computational Math: Numerical Methods course (APMA 4300)	<i>Fall 2019, Spring 2020</i>
Instructor - Academic Success Program - Introduction to Statistics course COLUMBIA UNIVERSITY	<i>Summer 2020, Summer 2021</i>
TA - Quantum Mechanics course (Chem 120A)	<i>Fall 2018, Spring 2019</i>
TA - General Chemistry course (Chem 1A)	<i>Summer 2018</i>
Head Tutor - College of Chemistry UNIVERSITY OF CALIFORNIA, BERKELEY	<i>Fall 2017 - May 2019</i>
Instructor - Workshop on Chemical Process Control and Dynamics TUMO CENTER FOR CREATIVE TECHNOLOGIES, YEREVAN, ARMENIA	<i>Winter 2019</i>

Scholarships

Graduate Excellence Scholarship - Armenian Professional Society	<i>2020</i>
Chevron Scholarship - University of California, Berkeley	<i>2019</i>
T.Z. and Irmgard Chu Scholarship - University of California, Berkeley	<i>2018</i>
John M. Azarian Memorial Armenian Youth Scholarship	<i>2018</i>
Harut Barsamian Scholarship	<i>2018</i>
Hrayr Terzian Alumni Scholarship - University of California, Berkeley	<i>2017</i>
Margarian Scholarship for Excellence in Education	<i>2017</i>
Koomruian Educational Fund Scholarship	<i>2017</i>

Armenian Relief Society Scholarship	2016 - 2018
Jack Arpajian Educational Foundation Scholarship	2016 - 2019
Luys Foundation Scholarship	2015 - 2019

Skills

ML Techniques	Variational Autoencoders, Computer Vision, Graph Neural Networks, Transformers, Gradient Boosting, Bayesian Optimization, Symbolic Regression
Programming/Technologies	Python (TensorFlow, PyTorch, Scikit-learn, Pandas, NumPy, Seaborn), SQL, MATLAB, Simulink, C++, Java, Git, Bash
Computational Simulations	DFT (VASP, Quantum ESPRESSO), Molecular Dynamics (LAMMPS), Monte Carlo, COMSOL, Aspen, Zemax, Synopsys Tools (Sentaurus), Pymatgen, AFLOW
Analytical Analysis Methods	HPLC, GC, FTIR, UV-VIS, NMR, MS, XRD
Languages	English, Russian, Armenian (working proficiency in all)

Selected Projects

Compartmental Models in Epidemiology Mar 2020 - June 2020

PYTHON

- Awarded a special prize for the paper by the President of The Republic of Armenia, Armen Sarkissian. [\[link\]](#)
- Modelled virus spread using compartmental models of different complexity and fitted to the country data of Armenia for future predictions on COVID-19 spread in the country.

Voice-Controlled Robotic Car Jan 2019 - May 2019

PYTHON, ENERGIA

- Implemented cluster formation algorithm for voice command recognition.
- Profiled motor behavior and operating conditions and designed a closed-loop control.
- Built the front-end circuitry for the car and denoised sound signals by adding a bias to improve the classification.

Google-Yelp Maps Nov 2016 - May 2017

PYTHON, JAVA

- Created an image rendering algorithm to enable zoom in/out.
- Interpreted data from an XML file into a recognizable graph-map form for the program.
- Implemented A* path-finding algorithm for navigation and designed rating-based Voronoi diagram for restaurants.

Design of an N-channel Silicon MOSFET Mar 2019 - May 2019

SENTAURUS DEVICE

- Optimized channel/body dopant concentration, junction depth and spacer length to achieve off current ≤ 1 nA per micron channel width and on current ≥ 400 μ A per micron channel width specifications.

Light-Fidelity (Li-Fi) Communications System Mar 2019 - May 2019

ZEMAX

- Built a Li-Fi transmitter: converted data to binary information and passed through high illumination LED.
- Built a Li-Fi receiver: used a photodiode receiver and an inverting amplifier to recover the original signal.
- Modelled an optical filter as a 4f system to select the necessary data, remove noise and potential corruptions.