Vahe Gharakhanyan

New York, NY

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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 and Research 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 the 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 patents (filed Oct. 2022, see below) for the 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 goal scoring, and simulating overall league standings using Monte Carlo method.
- Developed a ranking algorithm for predicting horse racing results from pairwise scores.

Columbia University, PI: Prof. Alexander Urban *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.
- 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.

UC Berkeley, PI: Prof. Mark Asta *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.

Publications and Patents(±)

- 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. (https://doi.org/10.1038/s41467-021-27154-2)
- Gadhiya, T., Shah, F., Vyas, N., **Gharakhanyan, V.**, Yang, J., and Holiday, A. (2022) Directional Variational Transformers for continuous molecular embedding. ELLIS ML4Molecules workshop. (jku.at)
- **Gharakhanyan, V.**, Wirth, L., Garrido Torres, J. A., Eisenberg, E., and Urban, A. (2022). Discovering melting-temperature prediction models of inorganic solids by combining supervised and unsupervised learning approaches. [in preparation]
- **Gharakhanyan, V.**,* Wang, T.,* Chatterjee, S., Trinkle, D., and Urban, A. (2022). ML-accelerated molecular dynamics simulations for predicting equilibrium melting points from short non-equilibrium simulations. (* 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]
- **Gharakhanyan, V.**, Yang, J., 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., **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., 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., **Gharakhanyan, V.** (2022). Molecular structure transformers for property prediction. *U.S. Patent App.*, filing date Oct 17, 2022. (±)

Presentations and Posters(±)

- Navigating materials design space with autoencoders to learn materials thermodynamics. APS March Meeting, March 2023, Las Vegas, NV. [upcoming]
- Machine learning and quantum-guided modeling of metal oxide thermodynamic properties. APS March Meeting, March 2023, Las Vegas, NV. [upcoming] (±)
- Learning materials similarity for the interpretation of thermodynamic properties with variational autoencoders. TMS Annual Meeting, March 2023, San Diego, CA. [upcoming]
- 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

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

Paper on Mathematical Modelling of Viruses, President's Special Award *Jun 2020*
President of The Republic of Armenia, Armen Sarkissian [*link*]

Design Competition: The Energy Transition Challenge, 2nd award *May 2018*
Chevron Corporation, Berkeley, CA

- Designed solar energy implementation into oil and gas company portfolios and inspired the global energy transition

Outstanding Tutor Award *Dec 2017*
University of California, Berkeley

President's Annual Award for the Best Student in Information Technology *Oct 2013*
Synopsys, Armenia

International Chemistry Olympiad 2012 and 2013, Two Bronze medals *Jul 2012, Jul 2013*
Washington DC, US and Moscow, Russia

Professional Service

Research Mentor - 2 Masters, 2 Undergraduate and 2 High-school students *2020 - Present*

Reviewer - AI4Mat workshop @ NeurIPS, Journal of Chemical Physics *2022 - Present*

Treasurer - Columbia Materials Advantage Student Chapter *2021 - 2022*

Scholarship Reviewer - UC Berkeley Achievement Award Program *May 2020*

Scholarship Reviewer - UC Berkeley Leadership Award Program *May 2020*

Jury Member - Baltic Chemistry Olympiad *2019 - 2020*

Team Member - Chemical Engineering Jeopardy, AIChE, UC Berkeley *2017 - 2019*

Volunteer - Wikimedia Armenia *2013 - 2015*

Teaching Experience

TA for Atomistic Simulations course (CHEN 4880) *Spring 2021*
Columbia University

TA for Computational Math: Numerical Methods course (APMA 4300) *Fall 2019, Spring 2020*
Columbia University

Instructor for Statistics course *Summer 2020, Summer 2021*
Academic Success Program, Columbia University

TA for Quantum Mechanics course (Chem 120A) *Fall 2018, Spring 2019*
University of California, Berkeley

Workshop on Chemical Process Control and Dynamics *Winter 2019*
Tumo Center for Creative Technologies, Yerevan, Armenia

TA for General Chemistry course (Chem 1A) *Summer 2018*
University of California, Berkeley

Head Tutor of Engineering, Science and Math courses *Fall 2017 - May 2019*
College of Chemistry, University of California, Berkeley

Scholarships

Armenian Professional Society Graduate Excellence Scholarship *2020*

Chevron Scholarship, University of California, Berkeley *2019*

T.Z. and Irmgard Chu Scholarship, University of California, Berkeley *2018*

John M. Azarian Memorial Armenian Youth Scholarship *2018*

Harut Barsamian Scholarship *2018*

Hrayr Terzian Alumni Scholarship, University of California, Berkeley *2017*

Margarian Scholarship for Excellence in Education *2017*

Koomruian Educational Fund Scholarship *2017*

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 μA 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.