Vahe Gharakhanyan

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Education

Columbia University *Aug 2019 - 2023*

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 - Apr 2023*

AI Resident (Generative Models for Materials Discovery, Computer Vision) *Mountain View, CA*

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

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.
- Created an end-to-end ML/quantum platform for molecular discovery for materials recycling applications.

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

- **Gharakhanyan, V.**, Aalto, M. S., Alsoulah, A., Artrith N., and Urban, A. (2023). Constructing and compressing global moment descriptors from local atomic environments. (2023). *The 11th International Conference on Learning Representations (ICLR 2023), ML4Materials workshop*. (*ml4materials.com*)
- 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.**, Chatterjee, S., Trinkle, D. R., Artrith N., and Urban, A. (2023). Constructing a compressed space of global representations from local atomic environments with information theory and autoencoders. [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.**, 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.**,† Aalto, M. S.,† and Urban, A. (2023). Quantifying the transferability of materials representations. († 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., and Holiday, A. (X Development LLC, 2023). Search for candidate molecules using quantum or thermodynamical simulations and autoencoder. *U.S. Patent Application 17/967,704*, June 1, 2023.
- Yang, J. H., **Gharakhanyan, V.**, Gadhiya, T., and Holiday, A. (X Development LLC, 2023). Ionic liquid-based depolymerization optimization. *U.S. Patent Application 17/967,711*, June 1, 2023.
- Gadhiya, T., Shah, F., Vyas, N., **Gharakhanyan, V.**, Yang, J. H., and Holiday, A. (X Development LLC, 2023). Depolymerization optimization platform. *U.S. Patent Application 17/967,723*, June 1, 2023.
- Gadhiya, T., Shah, F., Vyas, N., Yang, J. H., **Gharakhanyan, V.**, and Holiday, A. (X Development LLC, 2023). Molecular structure transformers for property prediction. *U.S. Patent Application 17/967,685*, June 1, 2023.
- Holiday, A., **Gharakhanyan, V.**, Gadhiya, T., Vyas, N., and Shah, F. (X Development LLC, 2023). Machine learning platform for finding solid catalysts for depolymerization reactions. *U.S. Provisional Patent Application 63/483,807*, filed Feb 8, 2023.

Presentations and Posters(†)

- Constructing and compressing global moment descriptors from local atomic environments. The 11th International Conference on Learning Representations (ICLR 2023), ML4Materials workshop, May 2023, Virtual, Kigali, Rwanda. (†)
- Materials representation learning with information-theory and variational autoencoders. Statistical Machine Learning Symposium, Columbia University, April 2023, New York, NY. (†)
- Constructing property-aware compressed materials representations with information-theory and autoencoders. Applied Physics and Applied Mathematics Research Symposium, Columbia University, April 2023, New York, NY.
- Constructing property-aware compressed materials representations. Data Science Day, Columbia University, April 2023, New York, NY. (†)
- 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. (†)
- 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. Data Science Day, Columbia University, April 2022, New York, NY. (†)

- Learning melting temperatures of binary materials with clustering and regression. Data Science Day, Columbia University, April 2022, New York, NY. (†)
- Combined clustering and regression for predicting melting temperatures of solids. 2022 TMS Annual Meeting, March 2022, Anaheim, CA.

Awards

IMPACT Award for Excellence in Graduate Research - Data Science Group
Distinguished Student Award - Forum on International Physics *Mar 2023*
Ovshinsky Student Prize - Division of Materials Physics
Energy Workshop Award - Group on Energy Research and Applications
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 *Jun 2020*
President of The Republic of Armenia - Armen Sarkissian [*press*]

2nd place - Design Competition: The Energy Transition Challenge *May 2018*
Chevron Corporation and UC Berkeley
- Designed solar energy implementation into oil and gas company portfolios and inspired the global energy transition.

Outstanding Tutor Award *Dec 2017*
College of Chemistry at UC Berkeley

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

Two Bronze medals - International Chemistry Olympiads 2012 and 2013 *Jul 2012, Jul 2013*
Washington DC, USA and Moscow, Russia

Professional Service

Research Mentor - 3 Masters, 2 Undergraduate and 2 High-school students *2020 - Present*

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

Research Mentor - Data Science Research Program @ The Coding School *2022 - 2023*

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

Scholarship Reviewer - UC Berkeley Achievement Award Program *2020*

Scholarship Reviewer - UC Berkeley Leadership Award Program *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 - Analysis of Engineering Problems course (CHEN 3020) *Spring 2023*
TA - Atomistic Simulations course (CHEN 4880) *Spring 2021*
TA - Computational Math: Numerical Methods course (APMA 4300) *Fall 2019, Spring 2020*
Instructor - Academic Success Program - Introduction to Statistics course *Summer 2020, Summer 2021*
Columbia University

TA - Quantum Mechanics course (Chem 120A) *Fall 2018, Spring 2019*
TA - General Chemistry course (Chem 1A) *Summer 2018*
Head Tutor - College of Chemistry *Fall 2017 - May 2019*
University of California, Berkeley

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

Scholarships

Graduate Excellence Scholarship - Armenian Professional Society *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.