

Vahe Gharakhanyan

RESEARCH ENGINEER AT META PLATFORMS, INC., FUNDAMENTAL AI RESEARCH [FAIR] CHEMISTRY TEAM

San Francisco, CA

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About

My expertise spans across computational materials science and chemistry, with a focus on new materials and molecular design and discovery using a combination of machine learning tools (like generative models) and computational materials science and chemistry methods, such as quantum (like Density Functional Theory [DFT]) and classical simulation methods (like Molecular Dynamics [MD]) to accelerate the transition to a more sustainable future (application areas include catalysis, display materials, recycling, and others).

I received a Ph.D. from Columbia University and a B.S. from UC Berkeley in related fields. In addition to academia, I have conducted industrial research on the same subjects at Google X, resulting in multiple patents and publications.

In November 2023, I joined Meta Platforms, Inc., the FAIR Chemistry team and our Open Catalyst Project initiative to work on the same topics with the primary focus of using machine learning and computational materials science and chemistry methods to accelerate novel materials/molecular design and discovery for a sustainable future, climate change solutions (catalysis, direct air capture), display materials, and other areas. The Open Catalyst Project is one of the world's most comprehensive and one-of-a-kind initiatives for accelerating materials design and discovery.

Education

Columbia University - New York, NY
Fu Foundation School of Engineering and Applied Science
Department of Applied Physics and Applied Mathematics

3 Sep 2019 - 15 May 2024

PHD MATERIALS SCIENCE AND ENGINEERING

GPA: 4.33 / 4.00

MPhil MATERIALS SCIENCE AND ENGINEERING

GPA: 4.33 / 4.00

MS MATERIALS SCIENCE AND ENGINEERING

GPA: 4.04 / 4.00

- MS conferred on 10 Feb 2021, MPhil conferred on 17 May 2023, and PhD conferred on 15 May 2024.
- Coursework: Machine Learning, Computational Math, Numerical Methods, Atomistic Simulations, Computing Electronic Structure, Phonon Calculations, Electric, Magnetic and Mechanical Properties, Crystallography.

University of California, Berkeley - Berkeley, CA
College of Engineering & College of Chemistry

19 Aug 2015 - 17 May 2019

BS MATERIALS SCIENCE AND ENGINEERING

GPA: 3.61 / 4.00

BS CHEMICAL ENGINEERING

MINOR ELECTRICAL ENGINEERING AND COMPUTER SCIENCES

- 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.

Work Experience

Meta Platforms, Inc.

6 Nov 2023 - Present

RESEARCH ENGINEER

San Francisco, CA

- Fundamental AI Research [FAIR] Chemistry Team** and **Open Catalyst Project [opencatalystproject.org]** – the most extended and one-of-a-kind initiative that is accelerating today's materials design and discovery in the world.
- Machine learning and computational materials science and chemistry methods for accelerating novel materials/molecular discovery for a sustainable future, climate change solutions (catalysis, direct air capture), display materials, and other areas.

Google X (officially X - The Moonshot Factory)

22 Jun 2022 - 2 Sep 2022

10 Oct 2022 - 28 Apr 2023

RESIDENT AT X (GENERATIVE MODELS FOR MATERIALS DISCOVERY)

Mountain View, CA

- X is Alphabet's moonshot factory. I was working in the area of machine learning for materials recycling.
- Authored two patents and a workshop paper (see below) for applications related to materials discovery for catalysis.
- Created an end-to-end ML platform for new materials discovery for catalysis and materials recycling applications.
- Used machine learning tools (like generative models) and computational materials science and chemistry methods, such as quantum simulations (like Density Functional Theory [DFT]) and thermodynamic modeling techniques.

Google X (officially X - The Moonshot Factory)

10 May 2021 - 3 Sep 2021

17 Sep 2021 - 17 Dec 2021

RESIDENT AT X (GENERATIVE MODELS FOR MOLECULAR DISCOVERY)

Mountain View, CA

- Co-developed four patents (see below) for applications related to molecular discovery for solvation/materials-recycling.
- Created an end-to-end ML and quantum platform for molecular discovery for solvation and recycling applications.

The Quant Edge

Aug 2020 - Feb 2021

QUANTITATIVE RESEARCH INTERN (ML TRACK) [UNPAID]

New York, NY

- Machine learning for sports betting.
- 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

Alexander Urban Research Group at Columbia University

2019 - 2024

MACHINE LEARNING AND QUANTUM SIMULATIONS FOR NEW MATERIALS DISCOVERY WITH TARGET PROPERTIES FOR SUSTAINABILITY AND RECYCLING

New York, NY

- NSF-funded project [Award #1940290] on employing machine learning and computational chemistry techniques to accelerate new materials discovery and materials property predictions.
- Work involved using a combination of machine learning, quantum (DFT), and classical (MD) computation techniques.
- Employing generative models (variational autoencoders) 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 machine learning force-fields.

Mark Asta Research Group at UC Berkeley

2018 - 2019

QUANTUM MECHANICS FOR MATERIALS DEFECT THERMODYNAMICS

Berkeley, CA

- Quantum simulations with density functional theory (DFT) for materials defect thermodynamics studies in TiO₂.

Publications

- **Gharakhanyan, V.** (2024). Advancing computational high-temperature materials thermodynamics with machine learning. *Doctoral dissertation, Columbia University*. doi.org/10.7916/1qnv-6142
- **Gharakhanyan, V.**, Wirth, L., Garrido Torres, J. A., Eisenberg, E., Wang, T., Trinkle, D. R., Chatterjee, S., and Urban, A. (2023). Discovering melting temperature prediction models of inorganic solids by combining supervised and unsupervised learning. *The Journal of Chemical Physics*, 160(20). doi.org/10.1063/5.0207033
- 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. nature.com/articles/s41467-021-27154-2 [in press]
- **Gharakhanyan, V.**, Aalto, M. S., Alsoulah, A., Artrith, N., and Urban, A. (2023). Constructing and compressing global moment descriptors from local atomic environments. *The 11th International Conference on Learning Representations (ICLR 2023), Machine Learning for Materials (ML4Materials) workshop*. openreview.net
- Gadhiya, T., Shah, F., Vyas, N., **Gharakhanyan, V.**, Yang, J. H., and Holiday, A. (2022). Directional Variational Transformers for continuous molecular embedding. *ELLIS 2022, Machine Learning for Molecules (ML4Molecules) workshop*. jku.at
- Boromand, A., Childress, K., Deshmukh, P., Fritzsche, C., Goyal, S., Hocker, J., Lan, J., Rao, T., Agrawal, A., Barroso-Luque, L., Bernat, V., **Gharakhanyan, V.**, Alvi, S., Carman, L. M., Abhishek, D., Hofmeyer, S., Levine, D. S., Liu, Z., Kulesa, C., Nie, Z., Reber, L., Rizvi, A., Diaz, L. R., Von Essen, C., Zhang, X., Harding, R., Klasen-Memmer, M., Uyttendaele, M., Ye, S., Zaitseva, N., Zitnick, C. L., Purvis, L., Ulissi, Z. W., and Ouderkirk, A. J. (2024). Organic solid crystal optical materials from concept to scalable devices. [submitted]
- Zhou, J., Huang, Y., Boromand, A., Zhang, X.*, **Gharakhanyan, V.*** (2024). Computational discovery of novel high refractive index liquid crystal polymers. [in preparation]
- **Gharakhanyan, V.**, Wang, T., Ramesh, S., Chatterjee, S., Trinkle, D. R., and Urban, A. (2025). ML-accelerated molecular dynamics simulations for predicting equilibrium melting points from short non-equilibrium simulations. [in preparation]
- Wirth, L., **Gharakhanyan, V.**, Thompson, M., Lu, Z., Wang, T., Gonzalez, D., Chatterjee, S., Urban, A., and Trinkle, D. R. (2025). 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.
- Holiday, A., **Gharakhanyan, V.**, Shah, F., Vyas, N., and Gadhiya, T. (X Development LLC, 2024). Machine learning platform for finding solid catalysts for depolymerization reactions. *U.S. Patent Application 18/435,957*, August 8, 2024.
- 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.**, Shah, F., Vyas, N., and Gadhiya, T. (X Development LLC, 2023). Machine learning platform for generating solid catalysts for depolymerization reactions. *U.S. Provisional Patent Application 63/509,220*, filed June 20, 2023.

Presentations and Posters(†)

- Crystal structure prediction of organic crystals through machine learning. Meta Reality Labs Fall 2024 Symposium, Nov 2024, Bellevue, WA. [upcoming] (†)
- Demo of materials science and chemistry machine learning and quantum mechanical workflow orchestrations. Meta Fundamental AI Research (FAIR) Conference 2024, Oct 2024, New York, NY. [upcoming]
- Crystal structure prediction of organic crystals through machine learning. Meta Fundamental AI Research (FAIR) Conference 2024, Nov 2024, New York, NY. [upcoming] (†)
- 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, Apr 2023, New York, NY. (†)
- Constructing property-aware compressed materials representations with information-theory and autoencoders. Applied Physics and Applied Mathematics Research Symposium, Columbia University, Apr 2023, New York, NY.
- Constructing property-aware compressed materials representations. Data Science Day, Columbia University, Apr 2023, New York, NY. (†)
- Navigating materials design space with autoencoders to learn materials thermodynamics. APS March Meeting, Mar 2023, Las Vegas, NV. ui.adsabs.harvard.edu/abs/2023APS..MARA53010G/abstract
- Machine learning and quantum-guided modeling of metal oxide thermodynamic properties. APS March Meeting, Mar 2023, Las Vegas, NV. (†) ui.adsabs.harvard.edu/abs/2023APS..MART00292G/abstract
- Machine learning and quantum-guided modeling of metal oxide thermodynamic properties. AIChE 4th Battery and Energy Storage Conference, The City College of New York, Oct 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, Sep 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, Jul 2022, Virtual. (†)
- Predicting melting temperatures of solids with combined clustering and regression. Artificial Intelligence for Materials Science (AIMS) Workshop, Jul 2022, Virtual. (†)
- High-temperature chemical reactions with ML-augmented first-principles computations. Data Science Day, Columbia University, Apr 2022, New York, NY. (†)
- Learning melting temperatures of binary materials with clustering and regression. Data Science Day, Columbia University, Apr 2022, New York, NY. (†)
- Combined clustering and regression for predicting melting temperatures of solids. 2022 TMS Annual Meeting, Mar 2022, Anaheim, CA.

Awards

IMPACT Award for Excellence in Graduate Research AMERICAN PHYSICAL SOCIETY - GROUP ON DATA SCIENCE	Mar 2023
Distinguished Student Award AMERICAN PHYSICAL SOCIETY - FORUM ON INTERNATIONAL PHYSICS	Mar 2023
Ovshinsky Student Prize AMERICAN PHYSICAL SOCIETY - DIVISION OF MATERIALS PHYSICS	Mar 2023
Energy Workshop Award AMERICAN PHYSICAL SOCIETY - GROUP ON ENERGY RESEARCH AND APPLICATIONS	Mar 2023
NSF Conference Fellowship MECHANISTIC ML AND DIGITAL TWINS (MMLDT-CSET) 2021 CONFERENCE	Jul 2021
Data Science/Medical Research Program Fellowship TECHFOUNDATION & HARVARD MEDICAL SCHOOL	Jul 2020
President's Special Award - Paper on Mathematical Modeling of Viruses PRESIDENT OF ARMENIA - ARMEN SARKISSIAN [<i>in press</i>]	Jun 2020
<ul style="list-style-type: none">Received a special prize from the President of Armenia, Armen Sarkissian, for my paper on the mathematical modeling of viruses, titled "Compartmental Models in Epidemiology: From SIR to ...S...I...R...".	
2nd place - Design Competition: The Energy Transition Challenge CHEVRON CORPORATION AND UC BERKELEY	May 2018
<ul style="list-style-type: none">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	Dec 2017
President's Annual Award for the Best Student in Information Technology SYNOPTIS & PRESIDENT OF ARMENIA - SERZH SARGSYAN [<i>in press</i>]	Oct 2013
Two Bronze medals - 44th and 45th International Chemistry Olympiads WASHINGTON, D.C., USA [<i>2012 U.S. Senate resolution 491</i>] AND MOSCOW, RUSSIA	Jul 2012, Jul 2013
Several National and Regional Olympiad Prizes (I, II, and III place awards) CHEMISTRY OLYMPIADS IN ARMENIA	Before 2013

Professional Service

Invited Member (one of initial 180 [now 229]) <i>autonomous-discovery.lbl.gov</i> CASE: THE COMMUNITY FOR AUTONOMOUS SCIENTIFIC EXPERIMENTATION	2022 - Present
Career Mentor - DataPoint Armenia K-minds program	Jul 2024
Scholarship Reviewer - Huys Foundation Scholarships	Jul 2024
Research Mentor - 3 MS, 2 UGrad, 3 HS [paper contributions available] <ul style="list-style-type: none">Max S. Aalto [PhD @ MIT], Ting Wang [PhD @ UCSD], Aminah Alsoulah, Sapna Ramesh [PhD @ Northwestern]David Gonzalez Jr., Ethan Eisenberg [UGrad @ UPenn], Daniel Sheinin [UGrad @ Georgia Tech], Amy Lin	2020 - 2023
Paper Reviewer <ul style="list-style-type: none">Peer-reviewed Journals: RSC Adv., J. Chem. Theory Comput., J. Chem. Phys.AI4Science Workshops: ML4PS @ NIPS 2024 & 2023 AI4Mat @ NIPS 2022 - 2024, BOKU 2024 ML4LMS @ ICML 2024	2022 - Present
Memberships (current and past) <ul style="list-style-type: none">Materials Research Society [MRS], American Physical Society [APS], The Minerals, Metals & Materials Society [TMS], American Institute of Chemical Engineers [AIChE]	2018 - Present
Research Mentor DATA SCIENCE RESEARCH PROGRAM @ THE CODING SCHOOL <ul style="list-style-type: none">Supervised two cohorts of six students to carry out a machine learning project for materials science applications.	Summer 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 & Problem Creator - Baltic Chemistry Competition	2018 - 2020
Team Member - Chemical Engineering Jeopardy, AIChE, UC Berkeley	2017 - 2019
Organizing Committee Member, Secretary, and Head Mentor of Armenian Chemistry Team - 49th International Mendeleev Olympiad 2015	May 2015
Jury Member and Head Instructor - Armenian National Chemistry Olympiads and Team Preparation	2013 - 2015
Volunteer - Wikimedia Armenia	2013 - 2015
Volunteer - 4th International Conference of Young Scientists: Chemistry	Aug 2014

Teaching Experience

TA - Analysis of Chemical 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	Sep 2017 - May 2019
UNIVERSITY OF CALIFORNIA, BERKELEY	
Instructor - Workshop on Vision of STEM Degrees	Summer 2020
STEMGEN SCHOOL, VIRTUAL, YEREVAN, ARMENIA	
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

Programming/Technologies

Python (TensorFlow, PyTorch, Scikit-learn, Pandas, NumPy, Seaborn), SQL, MATLAB, Simulink, C++, Java, Git, Bash

Computational Materials/Chemistry

DFT (VASP, Quantum ESPRESSO), Molecular Dynamics (LAMMPS), COSMO-RS, Monte Carlo, COMSOL, Aspen, Zemax, Synopsys TCAD (Sentaurus)

Languages

English, Russian, Armenian (working proficiency in all)