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.

I am currently at 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 *3 Sep 2019 - 15 May 2024*
Fu Foundation School of Engineering and Applied Science
Department of Applied Physics and Applied Mathematics

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 *19 Aug 2015 - 17 May 2019*
College of Engineering & College of Chemistry

BS Materials Science and Engineering
BS Chemical Engineering *GPA: 3.61 / 4.00*
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. The project went public in 2024 x.company/blog/posts/moonshot-for-circularity.
- 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) *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 TiO_2.

Publications

- 1. Wood, B.M., Dzamba, M., Fu, X., Gao, M., Shuaibi, M., Barroso-Luque, L., Abdelmaqsoud, K., **Gharakhanyan, V.**, Kitchin, J.R., Levine, D.S., Michel, K., Sriram, A., Cohen, T., Das, A., Rizvi, A., Sahoo, S.J., Ulissi, Z.W., and Zitnick, C.L. (2025). UMA: A Family of Universal Models for Atoms. *arXiv preprint arXiv:2506.23971.* *arxiv.com* [submitted to *The Thirty-Ninth Conference on Neural Information Processing Systems (NeurIPS 2025)*] *[in press - 1, 2, and 3]*
- 2. Levine, D.S., Shuaibi, M., Spotte-Smith, E.W.C., Taylor, M.G., Hasyim, M.R., Michel, K., Batatia, I., Csányi, G., Dzamba, M., Eastman, P., Frey, N.C., Fu, X., **Gharakhanyan, V.**, Krishnapriyan, A.S., Rackers, J.A., Raja, S., Rizvi, A., Rosen, A.S., Ulissi, Z., Vargas, S., Zitnick, C.L., Blau, S.M., and Wood, B.M. (2025). The Open Molecules 2025 (OMol25) Dataset, Evaluations, and Models. *arXiv preprint arXiv:2505.08762.* *arxiv.com* *[in press - 1, 2, and 3]*
- 3. Zhou, J., Huang, Y., Boromand, A., Noori, K, Purvis, L., Oh, C., Lu, L., Ulissi, Z.W., **Gharakhanyan, V.***, and Zhang, X.* [* joint last author] (2025). Genetic algorithm-accelerated computational discovery of liquid crystal polymers with enhanced optical properties. *arXiv preprint arXiv:2505.13477.* [submitted to *RSC Advances*] *arxiv.com*
- 4. Joshi, C.K., Fu, X., Liao, Y.L., **Gharakhanyan, V.**, Miller, B.K., Sriram, A., and Ulissi, Z.W. (2025) All-atom diffusion transformers: Unified generative modelling of molecules and materials. *arXiv preprint arXiv:2503.03965.* [**Spotlight** at *AI for Materials (AI4Mat) workshop at The 13th International Conference on Learning Representations (ICLR 2024)* and accepted to *The 42nd International Conference on Machine Learning (ICML 2025)*] *openreview.com*
- 5. Abed, J., Kim, J., Shuaibi. M., Wander, B., Duijf, B., Mahesh, S., Lee, H., **Gharakhanyan, V.**, Hoogland, S., Irtem, E., Lan, J., Schouten, N., Vijayakumar, A.U., Hattrick-Simpers, J., Kitchin, J. R., Ulissi, Z.W., van Vugt, A., Sargent, E.H., Sinton, D., and Zitnick, C.L. (2024). Open Catalyst Experiments 2024 (OCx24): Bridging experiments and computational models. *arXiv preprint arXiv:2411.11783.* [submitted to *Nature*] *arxiv.com* *[in press - 1, 2, and 3]*
- 6. **Gharakhanyan, V.** (2024). Advancing computational high-temperature materials thermodynamics with machine learning. *Doctoral dissertation, Columbia University*. *doi.org/10.7916/1qnv-6142*
- 7. **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*
- 8. **Gharakhanyan, V.**, Aalto, M.S., Alsoulah, A., Artrith N., and Urban, A. (2023). Constructing and compressing global moment descriptors from local atomic environments. *Machine Learning for Materials (ML4Materials) workshop at The 11th International Conference on Learning Representations (ICLR 2023)*. *openreview.net*

- 9. Gadhiya, T., Shah, F., Vyas, N., **Gharakhanyan, V.**, Yang, J.H., and Holiday, A. (2022). Directional Variational Transformers for continuous molecular embedding. *Machine Learning for Molecules (ML4Molecules) workshop at ELLIS 2022*. *jku.at*
- 10. 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 - 1 and 2]*
- 11. Boromand, A., Childress, K., Deshmukh, P., Fritzsch, 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., Kulessa, 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. (2025). Organic solid crystal optical materials from concept to scalable devices. [submitted to *Nature*]
- 12. **Gharakhanyan, V.***, Yang, Y., Barroso-Luque, L., Shuaibi, M., Levine, D.S., Michel, K., Bernat, V., Dzamba, M., Fu, X., Gai, M., Liu, X., Noori, K., Purvis, L.J., Rao, T., Wood, B.M., Rizvi, A., Uyttendaele, M., Ouderkirk, A.J., Daraio, C., Zitnick, C.L., Boromand, A., Marom, N., Ulissi, Z.W., and Sriram, A.* [* equal contribution] (2025). FastCSP: Accelerated molecular crystal structure prediction with Universal Model for Atoms. [to be posted to *arxiv* in July 2025]
- 13. **Gharakhanyan, V.**, Barroso-Luque, L., Yang, Y., Shuaibi, M., Michel, K., Levine, D.S., Dzamba, M., Fu, X., Gao, M., Liu, X., Ni, H., Noori, K., Wood, B.M., Uyttendaele, M., Boromand, A., Zitnick, C.L., Marom, N., Ulissi, Z.W., and Sriram, A. (2025). Open Molecular Crystals 2025 (OMC25) dataset and models. [to be posted to *arxiv* and submitted to *Scientific Data* in July 2025]
- 14. **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]
- 15. 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

- 1. **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 12,291,608***, issued May 6, 2025.
- 2. 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.
- 3. 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.
- 4. 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.
- 5. 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.
- 6. 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.
- 7. **Gharakhanyan, V.**, Purvis, L., Zhang, X., Boromand, A., Oh, C., Ulissi, Z.W., and Noori, K. (Meta Platforms, Inc., 2025). Genetic algorithm-accelerated computational discovery of liquid crystal polymers. *U.S. Provisional Patent Application 63/814,363*, filed May 29, 2025.

Presentations and Posters(†)

- ML-accelerated organic crystal structure prediction for next-gen optics. Meta Reality Labs Fall 2024 Symposium, Nov 2024, Bellevue, WA. (†)
- Demo of materials science and chemistry workflows. Meta Fundamental AI Research (FAIR) Conference 2024, Oct 2024, New York, NY.
- Crystal Clear: AI predicts crystal structures & optics. Meta Fundamental AI Research (FAIR) Conference 2024, Oct 2024, New York, NY. (†)

- 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 *Mar 2023*
American Physical Society - Group on Data Science

Distinguished Student Award *Mar 2023*
American Physical Society - Forum on International Physics

Ovshinsky Student Prize *Mar 2023*
American Physical Society - Division of Materials Physics

Energy Workshop Award *Mar 2023*
American Physical Society - Group on Energy Research and Applications

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 Modeling of Viruses *Jun 2020*
President of Armenia - Armen Sarkissian [*in press*]

- 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 *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 & President of Armenia - Serzh Sargsyan [*in press*]

Two Bronze medals - 44th and 45th International Chemistry Olympiads *Jul 2012, Jul 2013*
Washington, D.C., USA [*2012 U.S. Senate resolution 491*] and Moscow, Russia

Several National and Regional Olympiad Prizes (I, II, and III place awards) *Before 2013*
Chemistry olympiads in Armenia

Professional Service

Invited Member (one of initial 180 [now 229]) **autonomous-discovery.lbl.gov** *2022 - Present*
CASE: The Community for Autonomous Scientific Experimentation

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] *2020 - 2023*
- 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

Paper Reviewer *2022 - Present*
- Peer-reviewed Journals: RSC Adv., J. Chem. Theory Comput., J. Chem. Phys.
- Conferences & Workshops: AI4Mat @ ICLR 2025, NIPS 2022 - 2024, BOKU 2024 | ML4PS @ NIPS 2024 & 2023 | ML4LMS @ ICML 2024

Memberships (current and past) *2018 - Present*
- American Chemical Society [ACS], The Minerals, Metals & Materials Society [TMS], Materials Research Society [MRS], American Physical Society [APS], American Institute of Chemical Engineers [AIChE]

Research Mentor *Summer 2022 & 2023*
Data Science Research Program @ The Coding School
- Supervised two cohorts of six students to carry out a machine learning project for materials science applications.

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)