

Vahe Gharakhanyan

New York, NY

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Education

Columbia University

August 2019 - present

PHD MATERIALS SCIENCE AND ENGINEERING

GPA: 4.04 / 4.00

- Relevant Coursework: Machine Learning, Atomistic Simulations, Computing Electronic Structure, Phonon Calculations, Electric and Magnetic Properties, Mechanical Properties, Crystallography, Thermodynamics and Kinetics.

University of California, Berkeley

August 2015 - May 2019

BS MATERIALS SCIENCE AND ENGINEERING, BS CHEMICAL ENGINEERING

Minor Electrical Engineering and Computer Sciences

GPA: 3.61 / 4.00

- 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.

Work and Research Experience

AI Resident - Chemical Reaction Optimization with Machine Learning

May 2021 - September 2021

X - THE MOONSHOT FACTORY (FORMERLY Google[x]), MOUNTAIN VIEW, CA

- X is Alphabet's moonshot factory. The mission is to invent and launch moonshot technologies that make the world a radically better place. I am part of an early stage, confidential team.

Quantitative Research Intern - Machine Learning

August 2020 - February 2021

THE QUANT EDGE, NEW YORK, NY

- Worked towards predicting soccer match results using a team-strength metric and a Poisson model for goal scoring.
- Developed a machine learning method for predicting horse racing results by examining each pair of participants using Random Forest Classification.

Machine Learning for Optimization of Battery Devices for Energy Storage

October 2019 - present

SUPERVISOR: PROF. ALEXANDER URBAN, COLUMBIA UNIVERSITY

- Working towards using symbolic regression to understand different forms of melting within clusters of materials.
- Working towards learning about different forms of melting from short-time molecular dynamics (MD) simulations.
- Engineered features to allow for element permutations by including mathematical moments of physical parameters.
- Used Graph Neural Network (GNN) architecture for materials (MEGNet) to predict melting points of materials.

Density Functional Theory for Properties of Charged Defects

March 2018 - May 2019

SUPERVISOR: PROF. MARK ASTA, UNIVERSITY OF CALIFORNIA, BERKELEY

- 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

- J.A.G. Torres, **V. Gharakhanyan**, N. Artrith, T.H. Eegholm and A. Urban (2021). Predicting chemical reactions at high temperatures with machine learning and 0-Kelvin quantum mechanics. [in revision for *Nat. Commun.*]
- **V. Gharakhanyan**, J.A.G. Torres, E. Eisenberg and A. Urban (2021). Boosting Prediction of Melting Temperatures with Clustering. [in preparation]

Presentations

- Combined Clustering and Regression for Predicting Melting Temperatures of Solids.
2022 TMS Annual Meeting, March 2022, Anaheim, CA.
- Predicting Melting Temperatures of Solids via a Combined Model based on Clustering and Regression.
2021 MRS Fall Meeting, December 2021, Boston, MA.

Awards

NSF Conference Fellowship

July 2021

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

Data Science/Medical Research Program Fellowship

July 2020

TECHFOUNDATION, HARVARD MEDICAL SCHOOL

Paper on Mathematical Modelling of Viruses, President's Special Award June 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 December 2017
UNIVERSITY OF CALIFORNIA, BERKELEY

President's Annual Award for the Best Student in Information Technology October 2013
SYNOPSIS, ARMENIA

International Chemistry Olympiad 2012 and 2013, Two Bronze medals June 2012 - June 2013
WASHINGTON DC, US AND MOSCOW, RUSSIA

Leadership Experience

Treasurer - Columbia Materials Advantage Student Chapter August 2021 - May 2022

UC Berkeley Achievement Award Program Scholarship Reviewer May 2020

UC Berkeley Leadership Award Program Scholarship Reviewer May 2020

Jury Member - Baltic Chemistry Olympiad 2019 - 2020

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

Volunteer - Wikimedia Armenia 2013 - 2015

Scholarships

Armenian Professional Society Graduate Excellence Scholarship October 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

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

Skills

Programming/Technologies

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

Computational Simulations

DFT (Quantum ESPRESSO, VASP), Molecular Dynamics, Monte Carlo, LAMMPS, AFLOW, Pymatgen, COMSOL, Zemax, Synopsys Tools (Sentaurus), Aspen

Analytical Analysis Methods

HPLC, GC, FTIR, UV-VIS, NMR, MS, XRD

Languages

English, Russian, Armenian (working proficiency in all)

Programming Projects

Compartmental Models in Epidemiology

March 2020 - June 2020

PYTHON

- Awarded a special prize for the work 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.

Predicting Taxi Ride Duration in New York City

March 2019 - May 2019

PYTHON

- Performed data selection and cleaning by assessing the impact of a historical event (January 2016 US blizzard).
- Used Principal Component Analysis (PCA) to divide up the map of Manhattan into three equipartitioned regions.
- Validated the performance of the linear regression model and used tree regression on categorical variables.

Voice-Controlled Robotic Car

January 2019 - May 2019

PYTHON, ENERGIA

- Profiled motor behavior and operating conditions and designed a closed-loop control.
- Applied Principal Component Analysis (PCA) on voice commands and implemented cluster formation algorithm.
- Built the front-end circuitry for the car and denoised sound signals by adding a bias to improve the classification.

Google-Yelp Maps

An algorithm to recommend best restaurants based on user's ratings and location

November 2016 - May 2017

PYTHON, JAVA

- Created an image rendering algorithm to enable zoom in/out
- Interpreted data from xml file into a recognizable graph-map form for the program
- Implemented A* path-finding algorithm to find the shortest distance between two points
- Designed Voronoi diagram for restaurants that represents K-means unsupervised learning method for clustering

Engineering Projects

Design of an N-channel Silicon MOSFET

March 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

March 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.

Control System for a Two-cut Splitter

March 2018 - May 2018

SIMULINK, MATLAB

- Designed Internal Model Control (IMC) system based on a nonlinear process model.
- Implemented cascade, feedforward/feedback controllers for quality control of bottoms and distillate concentrations.