

GUILLERMO VAZQUEZ

Ph.D. Candidate · Computational Material Scientist

College Station, TX

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[vzguille](#) [Google Scholar](#) [vzguille.me](#)

Summary

- 5+ years of experience in Materials Design from materials simulations and data analytics
- 7+ years of experience with Density Functional Theory (DFT).
- 8+ years of experience in Python and computational science most popular modules such as scikit-learn, pandas, Tensorflow, etc. Dexterity in various programming languages for computational science. (Matlab, C++, Javascript, R, FORTRAN, etc.)
- Fast growing author in academia with 150+ citations in 7 peer-reviewed (3 as first author) journal publications during my PhD. Expected to publish 4 more (1 as first author) during my last year.

Education

Texas A&M University

Ph.D. in Materials Science & Engineering

Autonomous University of Queretaro

B.S. Nanotechnology Engineering

Aug. 2019 – Graduation Date: Aug 2024

College Station, TX

Aug. 2013 – Aug 2018

Queretaro, Mexico

Skills

Programming Languages: Python, Matlab, C++, Javascript, R, FORTRAN, SQL

Framework/OSs: GitHub, Windows, Linux, MacOS

Scientific Software: VASP, QuantumEspresso, VESTA, Xcrysden, Thermo-Calc, Origin, Gnuplot, Pandas, spaCy, scikit-learn, pyTorch, TensorFlow, OpenCV

Languages: English, Spanish

Experience

Texas A&M University

Research Assistant

Aug. 2019 – Aug. 2024

College Station, Texas

- Applied data analysis and machine learning methods such as feature engineering, classification, regression, validation, and optimization to experimental, literature compiled, and simulated materials design space.
- Generated a high-throughput DFT database generator framework for different configuration structures in an alloy system. Trained a GNN regression model for the application of commonly expensive DFT tasks.
- Used the CALPHAD method to generate millions of data points in a parallel high-throughput manner. Fitted to a Deep Neural Network regression model of custom architecture and used as a kernel in Bayesian and Particle Optimization for Material Design.
- Developed DFT automation methodologies for elastic and stability analysis in high dimensional alloy spaces.

Texas A&M University
Teaching Assistant

Aug. 2022 – May 2024
College Station, Texas

- **Fall 2022 Thermodynamics in Materials Science · Graduate level**
- **Spring 2023 and Spring 2024 Thermodynamics of Materials · Undergraduate level**
- Taught Thermodynamics at both the graduate and undergraduate levels, where I developed innovative problems and interactive lessons. These contributions are designed to benefit future generations at Texas A&M after I graduate.
- Created a Thermo-Calc walkthrough designed for undergraduate engineering students.
- Recipient of the Materials Science and Engineering Outstanding Teacher award.

Selected Publications

... for a complete list see my  [Google Scholar](#)

Efficient machine-learning model for fast assessment of elastic properties of high-entropy alloys.

Vazquez, G. et al., Singh, P., Saucedo, D., Couperthwaite, R., Britt, N., Youssef, K., Johnson, D.D. and Arróyave, R., 2022. *Acta Materialia*, 232, p.117924.

A deep neural network regressor for phase constitution estimation in the high entropy alloy system Al-Co-Cr-Fe-Mn-Nb-Ni. Vazquez, G., Chakravarty, S., Gurrola, R. and Arróyave, R., 2023. *npj Computational Materials*, 9(1), p.68.

Selected Presentations

Cluster Expansion Approximation Accelerated by a Graph Neural Network Regressor.
Vazquez, G., Saucedo, D., and Arroyave, R., Orlando, Florida, Mar. 2024

Deep Neural Network Regressor for Phase Fraction Estimation on the High Entropy Alloy System Al-Co-Cr-Fe-Mn-Nb-Ni. Vazquez, G., Chakravarty, S., Gurrola, R. and Arroyave, R., Anaheim, California, Feb. 2022

Honors & Awards

Datathon 2023 Texas A&M University Major League Hacking DATATHON 2023, 2nd place in Computer Vision Challenge **Oct. 2023**

Outstanding Teacher Department of Materials Science & Engineering Awards for my outstanding work as a TA in the MSEN 210 Course. **May 2023**

D3EM Certificate Recipient Accepted for the Data-Enabled Discovery and Design of Energy Materials (D3EM) Certificate. **Jun. 2020**

Prof. Development & Certifications

SATA 2022 - School for Advanced thermodynamics Assessments	Jun. 2022
1st Online VASP Workshop: Introduction to Ab-initio Simulation	Nov. 2021
Computational Materials Science Summer School 2021	Jun. 2021
AFLOW Summer School on Computational Materials Science Across Scales	Jun. 2020

Extracurricular Activities

ESL Teacher and IRA Volunteer at the Brazos Interfaith Immigration Network **Jan. - Jul. 2024**