

# GUILLERMO VAZQUEZ

Ph.D. Candidate · Computational Material Scientist

College Station, TX

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[vzguille.me](http://vzguille.me)

## Summary

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- 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.)
- 7+ years of experience with Density Functional Theory (DFT).
- 5+ years of experience in Materials Design from materials simulations and data analytics.
- 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

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**Texas A&M University**

*Ph.D. in Materials Science & Engineering*

**Aug. 2019 – Graduation Date: Aug 2024**

*College Station, TX*

**Autonomous University of Queretaro**

*B.S. Nanotechnology Engineering*

**Aug. 2013 – Aug 2018**

*Queretaro, Mexico*

## Experience

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**Texas A&M University**

*Research Assistant*

**Aug. 2019 – May 2024**

*College Station, Texas*

- Developed DFT automation methodologies for elastic and stability analysis in alloy spaces.
- Applied data analysis and machine learning to Materials Design.
- Used the CALPHAD method to calculate thousands of data points in a high-throughput manner. Fitted a regression model of custom architecture and used it as a kernel in optimization tasks for Material Design.
- Generated a high-throughput DFT database for different configuration structures in an alloy system. Trained a GNN regression model for the application of commonly expensive DFT tasks.

**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**
- Created a Thermo-Calc walkthrough designed for undergraduate engineering students.
- Created and graded challenging and comprehensive homework sets that helped the student approach thermodynamics from a Materials Science point of view.
- Recipient of the Materials Science and Engineering Outstanding Teacher award.

## Selected Publications

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### **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 Arroyave, 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 Arroyave, R., 2023. *npj Computational Materials*, 9(1), p.68.

## Selected Presentations

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**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

## Technical Skills

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**Programming Languages:** Python, Matlab, C++, Javascript, R, FORTRAN, SQL, HTML/CSS

**Framework/OSs:** GitHub, Windows, Linux, MacOS

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

**Languages:** English, Spanish

## Honors & Awards

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**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

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