

Guillermo Vazquez

PHD · COMPUTATIONAL MATERIALS SCIENTIST

College Station, Texas, USA

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Summary

- 5+ years of experience of Materials Design from materials simulations and data analytics. Expert in data analysis and machine learning methods such as feature engineering, classification, regression, validation, and optimization applied to experimental, literature compiled, and simulated materials design space.
- 7+ years of experience on Density Functional Theory (DFT).
- 8+ years of experience in Python and computational science most popular modules such as scikit-learn, scipy, pandas, TensorFlow, pyTorch, etc. Dexterity in various programming languages for computational science. (Matlab, C++, Javascript, R, FORTRAN, etc.)
- Fast growing author in academia with 200+ citations in 7 peer-reviewed (3 as first author) journal publications during my PhD. Expected to publish 3 more (1 as first author) during my last year.

Education

Texas A&M University

PHD IN MATERIALS SCIENCE AND ENGINEERING

- Advisor: Dr. Raymundo Arróyave.
- Materials Design via Ab Initio and Machine Learning methods.

College Station, Texas

Aug. 2019 - Aug. 2024

Autonomous University of Queretaro

B.S. IN NANOTECHNOLOGY ENGINEERING

- Honors thesis/Undergrad Research Advisor: Dr. Diego Espinosa
- Thesis: Development of a Special Quasirandom Structures (SQS) algorithm for alloy systems calculation for the Density Functional Theory method (DFT) (in Spanish)

Queretaro, Mexico

Aug. 2013 - Aug. 2018

Skills

Programming	Python, Matlab, C++, Javascript, R, FORTRAN, BASH, SQL, HTML/CSS
Operative Systems	LINUX, Windows, MacOS
Scientific Software	VASP, QuantumEspresso, VESTA, Xcrysden, Thermo-Calc, OpenCalphad, PANDAT, Gnuplot, Origin, Pandas, scikit-learn, scipy, matplotlib, spaCy, pyTorch, TensorFlow, OpenCV
Other Languages	Github, \LaTeX , Inkscape, Origin, Gnuplot, Word, PowerPoint, Excel English, Spanish

Teaching Experience

Thermodynamics of Materials

MSEN 210

- Filled in as substitute teacher on multiple occasions.
- Created a Thermo-Calc walk-through designed for engineering students at an undergrad level.
- Graded homework and papers for more than 60 students.

Texas A&M University

Jan. 2024 - May 2024

Thermodynamics of Materials

MSEN 210

- Created and graded a challenging yet comprehensive homework set that helped the student approach thermodynamics from a Materials Science point of view.
- Created online supporting material weekly.
- Held multiple office hours each week and offered personalized support to struggling students in a class of over 90 undergraduates.
- Graded homework and papers.

Texas A&M University

Jan. 2023 - May 2023

Thermodynamics in Materials Science

MSEN 640

Texas A&M University

Aug. 2022 - Dec. 2022

- Held multiple office hours a week, graded homework, and papers for more than 60 graduate students.

Mentoring

Texas A&M University

- Currently guiding a team of undergraduate students Capstone Project focusing on Machine Learning applied to next generation Magnetic Materials. (2023-24)
- I guided a team of undergraduate students through a Capstone Project in the development of high-temperature HEAs through the use of DFT modelling method, data visualization and regression models (2022-23).
- Student Mentor of National Science Foundation (NSF) Research Experiments for Undergraduate (REU) program twice (2021, 2022).

Research Experience

Texas A&M University

Computational Materials

Science Lab., College Station, TX.

Aug. 2019 - Present

- **High-Throughput DFT Calculation and Graph Neural Network Regressor Training.**
 - Conducted high-throughput (HT) runs of distinct structural configurations using DFT to build a comprehensive configuration database.
 - Trained and deployed a Graph Neural Network (GNN) surrogate model for HT relaxations.
 - Stress-strain elastic constant estimation comparison for DFT and GNN-assisted relaxer for a same system.
 - Cluster Expansion (CE) fitting and study of chemical ordering for an array of different HEAs.
- **NiTi-based High Entropy Shape Memory Alloys (HESMAs) design.**
 - HESMAs design through hysteresis optimization via Active Learning in a Batch Bayesian Optimization based framework.
 - Focused on DFT estimation for composition development of a CALPHAD-based TDB for the BCC/B19' lattice in NiTi-based Shape Memory Alloys.
 - Mentored the creation of a thermodynamic properties SMA ML model and high dimensional data visualization.
 - Alloy space screening via CALPHAD-ThermoCalc for single solid solution BCC.
- **Phase Constitution Estimation for a High Entropy System Using a Deep Neural Network Regressor.**
 - Utilized the CALPHAD method via ThermoCalc for the calculation of millions of datapoints within a high entropy system.
 - Developed a custom architecture Deep Neural Network (DNN) regressor to estimate phase constitution.
 - ML model used as a surrogate in Bayesian and Particle Optimization (BO, PSO, respectively) algorithms for Material Design.
- **Phase Identification Active Learning.**
 - Developed a pseudo-ternary HT exploration and visualization for a phase profile database.
 - Employed Bayesian Active Learning (BAL) to significantly improve the efficiency and throughput of phase identification tasks.
- **Elastic Constants Model for High Entropy Alloys.**
 - Developed a database of stiffness constants through DFT calculations.
 - Implemented a state-of-the-art ML model to accelerate sampling of alloy space, enabling a exhaustive analysis of high entropy alloy elastic properties.
- **High Entropy Diboride System Analysis.**
 - Studied diboride coatings properties in the high entropy realm from a DFT-ensemble perspective.
 - Calculated properties such as energy and stiffness for various configurations using DFT, and approximated finite temperature properties through statistical methods.
- **ML Model for the Discovery of New Rare-Earth Materials.**
 - Developed a SISSO ML model for estimating formation energy, contributing to a larger rare-earth study using data provided by colleagues.
- **ML Model for Estimation of SFE Values in FCC High-Entropy Alloys.**
 - Conducted a study on FCC-stability using Stacking Fault Energy values calculated via DFT.
 - Contributed a ML-model for rapid estimation and feature importance analysis.

Center for Engineering and Industrial Development

Surface Engineering and
Advanced Manufacturing Lab.,
Querétaro, México
Aug. 2017 - Aug. 2019

- Conducted a Nitride system calculation using Density Functional Theory (DFT).
 - Developed an algorithm to generate structures simulating a random alloy environment in DFT. This project marked my initial exploration into computational materials science and served as the focal point of my [undergraduate thesis](#).

Honors & Awards

Oct., 2023	Texas A&M University Major League Hacking DATATHON 2023 , Computer Vision Challenge Winner, used Tensorflow to train a Convolutional Neural Network for pattern recognition.	College Station, Texas
May, 2023	Outstanding Teacher , Department of Materials Science & Engineering Awards for my outstanding work as a TA in the MSEN 210 Course.	College Station, Texas
Jun., 2020	D3EM Certificate Recipient , Recipient of the Data-Enabled Discovery and Design of Energy Materials (D3EM) Certificate .	College Station, Texas
Sep. 2015	Youth of Excellence , Prestigious Scholarship awarded to the brightest students in their undergrad class.	Queretaro, Mexico

Professional Development & Certificates

Jun., 2022	SATA 2022 - School for Advanced thermodynamics Assessments ,	Toulouse, France
Nov., 2021	1st Online VASP Workshop: Introduction to Ab-initio Simulation ,	Online
Jun. 2021	Computational Materials Science Summer School 2021, Texas A&M ,	College Station, Texas
Jun., 2020	AFLOW Summer School on Computational Materials Science Across Scales Texas A&M University 2020 ,	Online

Publications

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

VAZQUEZ, G., SARITURK, D., AND ARRÓYAVE, R.(2024). HIGH-THROUGHPUT EXPLORATION OF ORDERING IN THE BCC-FCC ALCoCrCuFeMnNiV HEA SYSTEM
In Progress

VAZQUEZ, G., KARAMAN, I., AND ARRÓYAVE, R.(2024). OPTIMIZATION METHODS TO ESTIMATE THE NiTiCuHf B19' PHASE LATTICE PARAMETERS VIA HT-DFT. *In Progress*

MINGZHOU, F., , **VAZQUEZ, G.**, ARRÓYAVE, R.(2024) AND QIAN, X. **BAYESIAN ACTIVE LEARNING TO ACCELERATE HIGH THROUGHPUT PHASE IDENTIFICATION.** *In Review*

BROUCEK, J., KHATAMSAZ, D., ÇAKIRHAN, C., ZADEH, S.H., FAN, M., **VAZQUEZ, G.**, ATLI, K.C., QIAN, X., ARRÓYAVE, R., KARAMAN, I., (2024). **DESIGN OF HIGH-TEMPERATURE NiTiCuHf SHAPE MEMORY ALLOYS WITH MINIMUM THERMAL HYSTERESIS USING BAYESIAN OPTIMIZATION.** *In Review*

VAZQUEZ, G., SAUCEDA, D., AND ARROYAVE, R.(2024). **DECIPHERING CHEMICAL ORDERING IN HIGH ENTROPY MATERIALS: A MACHINE LEARNING-ACCELERATED HIGH-THROUGHPUT CLUSTER EXPANSION APPROACH.** *Acta Materialia*
Pre-published [HTTPS://DOI.ORG/10.1016/J.ACTAMAT.2024.120137](https://doi.org/10.1016/j.actamat.2024.120137)

SAUCEDA, D., SINGH, P., FALKOWSKI, A.R., CHEN, Y., DOUNG, T., **VAZQUEZ, G.,** RADOVIC, M. AND ARROYAVE, R., (2021). **HIGH-THROUGHPUT REACTION ENGINEERING TO ASSESS THE OXIDATION STABILITY OF MAX PHASES.** *npj Computational Materials*, 7(1), pp.1-13.
[HTTPS://DOI.ORG/10.1038/S41524-020-00464-7](https://doi.org/10.1038/s41524-020-00464-7)

KHAN, T.Z., KIRK, T., **VAZQUEZ, G.,** SINGH, P., SMIRNOV, A.V., JOHNSON, D.D., YOUSSEF, K. AND ARROYAVE, R., (2022). **TOWARDS STACKING FAULT ENERGY ENGINEERING IN FCC HIGH ENTROPY ALLOYS.** *Acta Materialia*, 224, p.117472.
[HTTPS://DOI.ORG/10.1016/J.ACTAMAT.2021.117472](https://doi.org/10.1016/j.actamat.2021.117472)

SINGH, P., DEL ROSE, T., **VAZQUEZ, G.,** ARROYAVE, R. AND MUDRYK, Y., 2022. **MACHINE-LEARNING ENABLED THERMODYNAMIC MODEL FOR THE DESIGN OF NEW RARE-EARTH COMPOUNDS.** *Acta Materialia*, 229, p.117759.
[HTTPS://DOI.ORG/10.1016/J.ACTAMAT.2022.117759](https://doi.org/10.1016/j.actamat.2022.117759)

VAZQUEZ, G., SINGH, P., SAUCEDA, D., COUPERTHWAITE, R., BRITT, N., YOUSSEF, K., JOHNSON, D.D. AND ARROYAVE, R., (2022). **EFFICIENT MACHINE-LEARNING MODEL FOR FAST ASSESSMENT OF ELASTIC PROPERTIES OF HIGH-ENTROPY ALLOYS.** *Acta Materialia*, 232, p.117924. [HTTPS://DOI.ORG/10.1016/J.ACTAMAT.2022.117924](https://doi.org/10.1016/j.actamat.2022.117924)

ZADEH, S.H., BEHBAHANIAN, A., BROUCEK, J., FAN, M., **VAZQUEZ, G.,** NOROOZI, M., TREHERN, W., QIAN, X., KARAMAN, I. AND ARROYAVE, R., 2023. **AN INTERPRETABLE BOOSTING-BASED PREDICTIVE MODEL FOR TRANSFORMATION TEMPERATURES OF SHAPE MEMORY ALLOYS.** *Computational Materials Science*, 226, p.112225.
[HTTPS://DOI.ORG/10.1016/J.COMMATSCI.2023.112225](https://doi.org/10.1016/j.commatsci.2023.112225)

VAZQUEZ, G., CHAKRAVARTY, S., GURROLA, R. AND ARROYAVE, R., 2023. **A DEEP NEURAL NETWORK REGRESSOR FOR PHASE CONSTITUTION ESTIMATION IN THE HIGH ENTROPY ALLOY SYSTEM AL-CO-CR-FE-MN-NB-NI.** *npj Computational Materials*, 9(1), p.68. [HTTPS://DOI.ORG/10.1038/S41524-023-01021-8](https://doi.org/10.1038/s41524-023-01021-8)

XIANG, Z., FAN, M., **VÁZQUEZ TOVAR, G.,** TREHERN, W., YOON, B.-J., QIAN, X., ARROYAVE, R., AND QIAN, X. (2021). **PHYSICS-CONSTRAINED AUTOMATIC FEATURE ENGINEERING FOR PREDICTIVE MODELING IN MATERIALS SCIENCE.** *Proceedings of the AAAI Conference on Artificial Intelligence*, 35(12), 10414-10421.
[HTTPS://DOI.ORG/10.1609/AAAI.V35I12.17247](https://doi.org/10.1609/aaai.v35i12.17247)

Presentations

TMS 2024 Annual Meeting & Exhibition

CLUSTER EXPANSION APPROXIMATION ACCELERATED BY A GRAPH NEURAL NETWORK REGRESSOR.

Vazquez, G., Saucedo, D., and Arroyave, R.,

Orlando, Florida

Mar. 2024

TMS 2023 Annual Meeting & Exhibition

DFT STUDY OF THE NiTi-X SYSTEMS FOR SHAPE MEMORY ALLOYS (SMAs) DESIGN.

Vazquez, G., Zadeh, S., Samanta, S., Van de Walle, A. and Arroyave, R.,

San Diego, California

Mar. 2023

TMS 2022 Annual Meeting & Exhibition

Anaheim, California

DEEP NEURAL NETWORK REGRESSOR FOR PHASE FRACTION ESTIMATION ON THE HIGH ENTROPY ALLOY SYSTEM AL-CO-CR-FE-MN-NB-NI.

Feb. 2022

Vazquez, G., Chakravarty, S., Gurrola, R. and Arroyave, R.,

TMS 2022 Annual Meeting & Exhibition

Anaheim, California

PHYSICS BASED ANALYTICAL MODELS FOR THE DESIGN OF NEW METASTABLE RARE-EARTH COMPOUNDS.

Feb. 2022

Singh, P., Del Rose, Vazquez, G., Arroyave, R., and Mudryk, Y.

TMS 2021 Annual Meeting & Exhibition

Orlando, Florida | Online

ELASTIC PROPERTIES MACHINE-LEARNING-BASED DESCRIPTOR FOR A REFRACTORY HIGH ENTROPY ALLOY.

Mar. 2021

Vazquez, G., Singh, P., Saucedo, D. and Arroyave, R.,

TMS 2021 Annual Meeting & Exhibition

Orlando, Florida | Online

USING MACHINE LEARNING FOR TARGETED ALLOY DESIGN IN HIGH ENTROPY COMPOSITION SPACES.

Mar. 2021

Kirk, T., Couperwaite, R., Vazquez, G., Saucedo, D., Honarmandi, P., Singh, P., and Arroyave, R.

Volunteer work

ESL Teacher at the Bryan Interfaith Immigration Network, Taught

Jan., 2024 English to Spanish speakers at the Bryan Interfaith Immigration Network in

- July 2024 Bryan, Texas. I additionally supported the community as an Information, Referrals, & Assistance volunteer.

Bryan, Texas