

Guillermo Vazquez

PHD STUDENT · 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.
- 6+ years of experience on 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 any programming language for computational science (Mat- lab, C++, JavaScript, R, FORTRAN, etc.).
- • Fast growing author in academia with 150+ citations in 7 peer-reviewed (3 first author) journal publications during my PhD. Expected to publish 4 more (1 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, BASH, MATLAB, C++, JavaScript, R, FORTRAN, SQL, HTML/CSS
Operative Systems	LINUX, Windows, MacOS
Scientific Software	VASP, QuantumEspresso, VESTA, Xcrysden, Thermo-Calc, OpenCalphad, PANDAT, Origin, Pandas, scikit-learn, pyTorch, TensorFlow, OpenCV
Other	Github, \LaTeX , Inkscape, Origin, Gnuplot, Word, PowerPoint, Excel
Languages	English, Spanish

Teaching Experience

Thermodynamics of Materials

MSEN 210

- Continued to expand on the work done the previous year, creating new class resources such as quizzes and homework for the next generations of engineers.
- Filled in as substitute teacher on multiple occasions.
- Created a Thermo-Calc walk-through designed for engineering students at an undergrad level.

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.
- Hold multiple office hours a week and a personal interest in struggling students in a class of more than 90 undergraduates.

Texas A&M University

Jan. 2023 - May 2023

Thermodynamics in Materials Science

MSEN 640

- Hold office hours, graded homework, and papers for more than 60 graduate students.

Texas A&M University

Aug. 2022 - Dec. 2022

- 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 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*

- **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 high-throughput 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.
- **Phase Constitution Estimation for a High Entropy System Using a Deep Neural Network Regressor.**
 - Utilized the CALPHAD method via ThermoCalc for high-throughput calculation of thousands of datapoints within a high entropy system.
 - Developed a custom architecture Deep Neural Network regressor to estimate phase constitution, applied in optimization tasks for Material Design.
- **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.
- **NiTi-based Shape Memory Alloys High-Throughput Analysis via DFT and ML.**
 - Primarily focused on DFT estimation for composition development of a CALPHAD-based TDB for the BCC/B19' lattice in NiTi-based Shape Memory Alloys.
 - Consulted for the development of the ML-model and alloy space screening via CALPHAD-ThermoCalc for single solid solution BCC.
- **High-Throughput DFT Calculation and Graph Neural Network Regressor Training for Acceleration of Expensive DFT Frameworks for Metallic Alloys.**
 - Integrated DFT, ML, and the CALPHAD method for a comprehensive project during my PhD.
 - Conducted high-throughput runs of distinct structural configurations through DFT to replace it with a more efficient surrogate model for commonly expensive DFT tasks (to be published).

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 , Admitted for 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 ,	College Station, Texas
Jun., 2020	AFLOW Summer School on Computational Materials Science Across Scales Texas A&M University 2020 ,	Online

Publications

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*

VAZQUEZ, G., SAUCEDA, D., AND ARRÓYAVE, R.(2024). **DECIPHERING CHEMICAL ORDERING IN HIGH ENTROPY MATERIALS: A MACHINE LEARNING-ACCELERATED HIGH-THROUGHPUT CLUSTER EXPANSION APPROACH**. *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*

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 ARRÓYAVE, 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 ARRÓYAVE, 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 ARRÓYAVE, 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.

Orlando, Florida

Mar. 2024

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

TMS 2023 Annual Meeting & Exhibition

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

San Diego, California

Mar. 2023

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

TMS 2022 Annual Meeting & Exhibition

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

Anaheim, California

Feb. 2022

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

TMS 2022 Annual Meeting & Exhibition

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

Anaheim, California

Feb. 2022

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

TMS 2021 Annual Meeting & Exhibition

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

Orlando, Florida | Online

Mar. 2021

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

TMS 2021 Annual Meeting & Exhibition

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

Orlando, Florida | Online

Mar. 2021

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

Volunteer work

ESL Teacher at the Bryan Interfaith Immigration Network, Teaching English to Spanish speakers at the Jan., 2024 Bryan Interfaith Immigration Network in College Station, Texas, was a way for me to give back to the vibrant Texas community that welcomed me during my PhD years.

College Station,
Texas