# Guillermo **Vazquez**

PhD Student · Computational Materials Scientist
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## Summary


- 5+ years of experience of Materials Design from materials simulations and data analytics.
- 7+ years of experience on Density Functional Theory (DFT).
- 8+ years of experience on Python and computational science most popular modules such as: scikit-learn, pandas, Tensorflow, etc. Dexterity in any programming language for computational science (Matlab, 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** — *College Station, Texas*
PhD in Materials Science and Engineering — *Aug. 2019 - Aug. 2024*
- Advisor: Dr. Raymundo Arróyave.
- Materials Design via Ab Initio and Machine Learning methods.

**Autonomous University of Queretaro** — *Queretaro, Mexico*
B.S. in Nanotechnology Engineering — *Aug. 2013 - Aug. 2018*
- 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)

## Skills

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

## Teaching Experience

**Thermodynamics of Materials** — *Texas A&M University*
MSEN 210 — *Jan. 2024 - May 2024*
- 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.

**Thermodynamics of Materials** — *Texas A&M University*
MSEN 210 — *Jan. 2023 - May 2023*
- 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.

**Thermodynamics in Materials Science** — *Texas A&M University*
MSEN 640 — *Aug. 2022 - Dec. 202*
- Hold office hours, 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 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*

- (1) 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

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| 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**, Admited 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

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| 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

Mingzhou, F., **, Vazquez, G.**, Arróyave, R.(2024) and Qian, X. **Bayesian Active Learning to Accelerate High Throughput Phase Identification.** *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*

**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., Cakirhan, 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

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

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

**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

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

**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

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

## Presentations

**TMS 2024 Annual Meeting & Exhibition** — *Orlando, Florida* — *Mar. 2024*
Cluster Expansion Approximation Accelerated by a Graph Neural Network Regressor.
**Vazquez, G.**, Sauceda, D., and Arroyave, R.,

**TMS 2023 Annual Meeting & Exhibition** — *San Diego, California* — *Mar. 2023*
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.,

**TMS 2022 Annual Meeting & Exhibition** — *Anaheim, California* — *Feb. 2022*
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.,

**TMS 2022 Annual Meeting & Exhibition** — *Anaheim, California* — *Feb. 2022*
Physics Based Analytical Models for the Design of New Metastable Rare-earth Compounds.
Singh, P., Del Rose, **Vazquez, G.**, Arroyave, R., and Mudryk, Y.

**TMS 2021 Annual Meeting & Exhibition** — *Orlando, Florida | Online* — *Mar. 2021*
Elastic Properties Machine-Learning-based Descriptor for a Refractory High Entropy Alloy.
**Vazquez, G.**, Singh, P., Sauceda, D. and Arroyave, R.,

**TMS 2021 Annual Meeting & Exhibition** — *Orlando, Florida | Online* — *Mar. 2021*
Using Machine Learning for Targeted Alloy Design in High Entropy Composition Spaces.
Kirk, T., Coupertwaite, R., **Vazquez, G.**, Sauceda, D., Honarmandi, P., Singh, P., and Arroyave, R.

## Volunteer work

Jan., 2024 — **ESL Teacher at the Bryan Interfaith Immigration Network**, Teaching English to Spanish speakers at the 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*