Guillermo **Vazquez**

PhD Student · Computational Materials Scientist

College Station, Texas, USA

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| vzguille | vzguille | G Vazquez

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 in 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

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, spaCy pyTorch, TensorFlow, OpenCV
Other	Github, LaTeX, Inkscape, Origin, Gnuplot, Word, PowerPoint, Excel
Languages	English, Spanish

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

- High-Throughput DFT Calculation and Graph Neural Network Regressor Training for Acceleration of Expensive DFT Frameworks for Metallic Alloys.
  - Conducted high-throughput runs of distinct structural configurations through DFT to replace it with a more efficient surrogate model for commonly expensive DFT tasks.
- 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 millions 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.
- Shape Memory Alloy Design.
  - Experimental-theoretical Multidisciplinary Shape Memory Alloy design through hysteresis optimization via Active Learning in a Batch Bayesian Optimization based framework.
- 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.
- 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.

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**, 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

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.** *Acta Materialia Pre-published* https://doi.org/10.1016/j.actamat.2024.120137

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*