Guillermo **Vazquez**

PhD · Computational Materials Scientist
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| vzguille | vzguille | Google Scholar: G Vazquez

Summary

- Enthusiast Computational scientist with 8+ years of experience in materials design. Primary interests are Physics-informed Machine Learning, Active Learning, and Disordered Materials.
- 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 — *College Station, Texas*
PhD in Materials Science and Engineering — *Aug. 2019 - Aug. 2024*
- Advisor: Dr. Raymundo Arróyave.
- Thesis: Machine Learning and Ab Initio Study of High Entropy Systems.

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, Matlab, C++, Javascript, R, FORTRAN, BASH, SQL, HTML/CSS
Operative Systems	LINUX, Windows, MacOS
Scientific Software	VASP, QuantumEspresso, ASE, pymatgen, RDKit, LAMMPS, VESTA, Xcrysden, Thermo-Calc OpenCalphad, PANDAT, Origin, Gnuplot, Pandas, scikit-learn, scipy, matplotlib, spaCy, NLTK pyTorch, TensorFlow, OpenCV
Other	Github, Desktop, LaTeX, Inkscape, Origin, Gnuplot, Word, PowerPoint, Excel
Languages	Fluent Proficiency in English, Native Proficiency in Spanish

Teaching Experience

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

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.
- Held multiple office hours each week and offered personalized support to struggling students in a class of over 90 undergraduates.
- Graded homework and papers.

Thermodynamics in Materials Science *Texas A&M University*

MSEN 640 *Aug. 2022 - Dec. 202*

- 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**, Image Classification Challenge Winner, used Tensorflow to train a Convolutional Neural Network (CNN) for stroke 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

Aug, 2024	**Advanced NLP with Python for Machine Learning**,	*Online*
Aug, 2024	**LLaMa for Developers**,	*Online*
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*

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., 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*

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

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 - July 2024 **ESL Teacher at the Bryan Interfaith Immigration Network**, Taught English to Spanish speakers at the Bryan Interfaith Immigration Network in Bryan, Texas. I additionally supported the community as an Information, Referrals, & Assistance volunteer. *Bryan, Texas*