Guillermo **Vazquez**

PhD · Computational Materials Scientist
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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, Blender, 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. 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 - Aug. 2024

- 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., Queretaro, 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.

Work Experience

Independent

Austin, Texas
Sep. 2024 - currently

- DFT-ready environment containerization for Google Cloud Services.
  - Quantum Espresso wrapper code for high-throughput python based on the ASE module for ionic and cell relaxation workflows.
  - Environment containerization into the Google Artifact Registry.
  - Deployed via the Google Compute Engine to calculate thousands of structures added seamlessly to multi-platform access through Google Cloud SQL.

Domus Agency / M2Desarrollos

Queretaro, Mexico
Sep. 2018 - Jul. 2019

- Web Developer, Database Management, and IT Support Specialist.
  - Designed and maintained the company's website, and multiple user-oriented websites for real estate developments. Creating user-friendly interfaces and responsive design across different devices. (HTML, CSS, javascript)
  - Managed and maintained company real estate databases, including customer emails and internal company data (MySQL).
  - Acted as the go-to IT solutions provider for the company technical issues, ensuring smooth day-to-day operations for employees.

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*