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 100+ citations in 7 peer-reviewed (2 first author) journal publications during my PhD. Expected to publish 5 more (2 first author) during my last year.

Education

Texas A&M University — *College Station, Texas*
PhD in Materials Science and Engineering — *Aug. 2019 - May. 2024*
- Advisor: Dr. Raymundo Arróyave.

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, 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.
- 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.

Aug. 2019 - Present

- (1) Elastic constants model for High Entropy Alloys.
  Calculated a stifness constant database from DFT calculations . Then a state-of-the-art ML model was fitted into the data, accelerating sampling of the alloy space which allowed us to run a high-throughput analysis of the high entropy alloy elastic properties.
- (2) High Entropy diboride system analysis for aerospace industry.
  Diboride coatings properties in the high entropy realm are studied from a DFT-ensemble point of view. Where we calculate some configuration's properties, such as energy and stiffness) from DFT and we approximate a finite temperature approximation from a statistical approach.
- (3) Phase constitution estimation for a high entropy system using a Deep Neural Network Regressor.
  Using the CALPHAD method as implemented by ThermoCalc we calculate in a high-throughput manner thousands of datapoints inside a high entropy system. We then fit a Deep Neural Network regressor of custom architecture and proceed to use it as a kernel in optimization tasks for Material Design.
- (4) ML-model for the discovery of new rare-earth materials.
  Using data captured by colleagues I developed a SISSO ML model for the estimation of the formation energy as a contribution in a larger rare-earth study.
- (5) ML-model for the estimation of SFE values in FCC High-Entropy alloys.
  Stacking Fault Eenery values calculated via DFT are screened for a FCC-stability study. I contributed with a ML-model for quick estimation and feature importance analysis.
- (6) NiTi-based Shape Memory Alloys High-Throughput Analysis via DFT and ML.
  For this project, I worked mainly on the DFT estimation for compositions for the development of a CALPHAD-based TDB for the BCC/B19' lattice. I also participated as a consultant for the development of the ML-model and for the alloy space screening via CALPHAD-ThermoCalc for single solid solution. BCC
- (7) High-throughput DFT calculation and Graph Neural Network regressor training for the acceleration of expensive DFT frameworks for metallic alloys.
  This project encompasses all the work I did over my PhD (DFT, ML and the CALPHAD method). A high-throughput run of distinct configuration structures over DFT is carried over to ultimately replace it for a highly more efficient surrogate model for the application of commonly expensive DFT tasks (to be published).

Center for Engineering and Industrial Development

Surface Engineering and Advanced Manufacturing Lab.

Aug. 2017 - Aug. 2019

- (1) Nitride system calculation using Density Functional theory.
  Developed an algorithm for the generation of structure that mimic a random alloy enviroment in DFT. This was my first approach into computational science and the topic chosen for my undergraduate thesis.

Honors & Awards

Oct., 2023	**Texas A&M University Major League Hacking DATATHON 2023,** 2nd place in Computer Vision Challenge	*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,** Accepted 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., 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). **Cluster Expansion Approximation Accelerated by a Graph Neural Network Regressor.** *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 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 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 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 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

Feb, 2024 — **Mentor for the Youth of Excellence Program**, I work as a mentor for upcoming bright undergraduate students in Mexico looking to apply to high-quality international graduate programs. I return advice for my experience as a graduate student for those inclined towards US schools. — *Virtual*

Jan., 2024 — **ESL Teacher at the Bryan Interfaith Immigration Network**, As a part of the vibrant Texas community that hosted during my scientific developing years, I decided to give back to the community through the use of my language knowledge. — *College Station, Texas*