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 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
Operative Systems	LINUX, Windows, MacOS
Other	LaTeX, Inkscape, Origin, Gnuplot, Word, PowerPoint, Excel
Languages	Spanish, English

Teaching Experience

Thermodynamics in Materials Science — *Texas A&M University*

MSEN 640 — *Aug. 2022 - Dec. 202*

- Hold office hours, graded home-works, and papers for more than 60 graduate students.

Thermodynamics of Materials — *Texas A&M University*

MSEN 210 — *Jan. 2023 - May 2023*

- Created and graded challenging yet comprehensive homework set that helped the student approach thermodynamics from a Materials Science point of view.
- Created online supporting material in a weekly basis.
- Hold multiple office hours a week and a personal interest to struggling students in a class of more than 90 undergraduate students.

Mentoring — *Texas A&M University*

- Student Mentor of NSF Research Experiments for Undergraduate (REU) Program twice (2021, 2022).
- I guided a team of undergrads 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).

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

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*
Sep., 2019	**TAMU DATATHON 2019**,	*College Station, Texas*

Selected Publications

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

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

...See All

Presentations

TMS 2021 Annual Meeting & Exhibition — *Orlando, Florida | Online*

Elastic Properties Machine-Learning-based Descriptor for a Refractory High Entropy Alloy. — *Mar. 2021*

Vazquez, G., Singh, P., Sauceda, D. and Arroyave, R.,

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

Deep Neural Network Regressor for Phase Fraction Estimation on the High Entropy Alloy System Al-Co-Cr-Fe-Mn-Nb-Ni. — *Feb. 2022*

Vazquez, G., Chakravarty, S., Gurrola, R. and Arroyave, R.,

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

DFT study of the NiTi-X systems for Shape Memory Alloys (SMAs) design. — *Mar. 2023*

Vazquez, G., Zadeh, S., Samanta, S., Van de Walle, A. and Arroyave, R.,