

Guillermo Vazquez

PHD STUDENT · COMPUTATIONAL MATERIALS SCIENTIST

College Station, Texas, USA

☎ (+1) 979 739 66 89 | ✉ guillermo.vazquez@tamu.edu | 🌐 vzguille.me | 📷 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 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

PHD IN MATERIALS SCIENCE AND ENGINEERING

- Advisor: Dr. Raymundo Arróyave.

College Station, Texas

Aug. 2019 - May. 2024

Autonomous University of Queretaro

B.S. IN NANOTECHNOLOGY ENGINEERING

- 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)

Queretaro, Mexico

Aug. 2013 - Aug. 2018

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

MSEN 640

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

Texas A&M University

Aug. 2022 - Dec. 2022

Thermodynamics of Materials

MSEN 210

- 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.

Texas A&M University

Jan. 2023 - May 2023

Mentoring

- 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).

Texas A&M University

Research Experience

- **(1) Elastic constants model for High Entropy Alloys.**
Calculated a stiffness 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 Energy 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 environment in DFT. This was my first approach into computational science and the topic chosen for my undergraduate thesis.

Honors & Awards

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| 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

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| 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., COUPERTHWAIT, 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](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](https://doi.org/10.1038/s41524-023-01021-8)

[...See All](#)

Presentations

TMS 2021 Annual Meeting & Exhibition

ELASTIC PROPERTIES MACHINE-LEARNING-BASED DESCRIPTOR FOR A REFRACTORY HIGH ENTROPY ALLOY.

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

Orlando, Florida | Online

Mar. 2021

TMS 2022 Annual Meeting & Exhibition

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.,

Anaheim, California

Feb. 2022

TMS 2023 Annual Meeting & Exhibition

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.,

San Diego, California

Mar. 2023