

GUILLERMO VAZQUEZ

Ph.D. · Computational Material Scientist

College Station, TX

📞 +1 979-739-6689 ✉ guillermo.vazquez@tamu.edu 🌐 vzguille
📧 vzguille 🎓 Google Scholar: G Vazquez 🌐 vzguille.me

Enthusiastic computational materials scientist specializing in simulations and machine learning for materials. An emerging author with nine peer-reviewed publications and over 200 citations, my main interest are physics-informed machine learning, active learning, and disordered materials.

Education

Texas A&M University, College Station, TX

Aug 2019 – Aug 2024

Ph.D. in Materials Science & Engineering

GPA 3.75/4

Thesis: Machine Learning and Ab-initio Study of the Elastic and Thermodynamic Properties of High Entropy Systems.

Autonomous University of Queretaro, Queretaro, Mexico

Aug 2013 – Aug 2018

B.S. in Nanotechnology Engineering

GPA 3.6/4

Thesis: PSO algorithm for SQS generation.

Skills

Programming Languages: Python, Matlab, C++, HTML, CSS, Javascript, R, FORTRAN, SQL

Framework/OSs: GitHub, Docker, Windows, Linux, MacOS

Scientific Software: VASP, QuantumEspresso, ASE, pymatgen, RDKit, LAMMPS, VESTA, Xcrysden, Thermo-Calc, PANDAT, Origin, Gnuplot, Inkscape, Blender

Data Science and Programming: pandas, scipy, scikit-learn, Keras, TensorFlow, pyTorch, OpenCV, spaCy, NLTK

Languages: Fluent Proficiency in English, Native Proficiency in Spanish

Experience

Texas A&M University

Aug 2019 – Aug 2024

Research Assistant

College Station, Texas

- Applied **Data Science and Machine Learning methods** such as feature engineering, classification, regression, validation, and optimization to experimental, literature compiled, and simulated materials design space.
- Trained and published a **Machine Learning analytical model** (Sure Independent Screening and Sparsifying Operator) extrapolated from DFT calculated elastic constants.
- Collaborated in a **Computational-experimental multidisciplinary effort** to design Shape Memory Alloys through hysteresis optimization via Active Learning in a Batch Bayesian Optimization based framework.
- Led a **Big Data Phase Project** calculated via parallel high-throughput millions of phase fraction calculations. Then, used them to fit a Deep Neural Network (DNN) regression model of custom architecture and used as a kernel in Bayesian and Particle Optimization (BO, PSO, respectively) for Material Design.
- Created a **High-throughput Disordered DFT Database Generator and Calculation Framework** for different configuration structures in an alloy system. Trained a Graph Neural Network (GNN) regression model for commonly expensive DFT tasks. Including calculation of elastic and stability analysis in high dimensional alloy spaces.

- Mentored multiple young scientists including two undergraduate CAPSTONE projects, two REU students, and 3 graduate students.

Texas A&M University
Teaching Assistant

Aug 2022 – May 2024
College Station, Texas

- Fall 2022 Thermodynamics in Materials Science, Graduate level
- Spring 2023 and Spring 2024 Thermodynamics of Materials, Undergraduate level
- Developed innovative problems and interactive lessons for Thermodynamics Materials Science designed to benefit future generations at Texas A&M.
- Authored a Thermo-Calc walk-through designed for undergraduate engineering students.
- Recipient of the Materials Science and Engineering Outstanding Teacher award

Selected Publications

... for a complete list see my [Google Scholar](#)

Efficient machine-learning model for fast assessment of elastic properties of high-entropy alloys.

Vazquez, G. et al., Singh, P., Saucedo, D., Couperthwaite, R., Britt, N., Youssef, K., Johnson, D.D. and Arróyave, R., 2022. *Acta Materialia*, 232, p.117924.

A deep neural network regressor for phase constitution estimation in the high entropy alloy system Al-Co-Cr-Fe-Mn-Nb-Ni. Vazquez, G., Chakravarty, S., Gurrola, R. and Arróyave, R., 2023. *npj Computational Materials*, 9(1), p.68.

Selected Presentations

... for more see my [Academic CV](#)

Cluster Expansion Approximation Accelerated by a Graph Neural Network Regressor. Vazquez, G., Saucedo, D., and Arroyave, R. *at Orlando, Florida, TMS, Mar. 2024*

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. *at TMS, Anaheim, California, Feb. 2022*

Honors & Awards

Texas A&M University Major League Hacking DATATHON 2023 Image Classification Challenge award **Oct. 2023**

Outstanding Teacher [Department of Materials Science & Engineering Awards](#) for my outstanding work as a TA in the MSEN 210 Course. **May 2023**

D3EM Certificate Recipient Accepted for the Data-Enabled Discovery and Design of Energy Materials (D3EM) Certificate. **Jun. 2020**

Prof. Development & Certifications

Advanced NLP with Python for Machine Learning	Aug 2024
LLaMa for Developers	Aug 2024
SATA 2022 - School for Advanced thermodynamics Assessments	Jun 2022
1st Online VASP Workshop: Introduction to Ab-initio Simulation	Nov 2021
Computational Materials Science Summer School	Jun 2021
AFLOW Summer School on Computational Materials Science Across Scales	Jun 2020

Extracurricular Activities

ESL Teacher and IRA Volunteer at the Brazos Interfaith Immigration Network **Jan. - Jul. 2024**