Guillermo Vazquez

Ph.D. · Computational Material Scientist
College Station, TX
+1 979-739-6689 guillermo.vazquez@tamu.edu vzguille
vzguille Google Scholar vzguille.me

Summary

- 5+ years of experience in Materials Design from materials simulations and data analytics.
- 7+ years of experience with 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 4 more (1 as first author) during my last year.

Education

Texas A&M University **Aug. 2019 – Graduation Date: Aug 2024**
Ph.D. in Materials Science & Engineering *College Station, TX*
Autonomous University of Queretaro **Aug. 2013 – Aug 2018**
B.S. Nanotechnology Engineering *Queretaro, Mexico*

Skills

Programming Languages: Python, Matlab, C++, Javascript, R, FORTRAN, SQL
Framework/OSs: GitHub, Windows, Linux, MacOS
Scientific Software: VASP, QuantumEspresso, VESTA, Xcrysden, Thermo-Calc, Origin, Gnuplot, pandas, spaCy, scipy, scikit-learn, TensorFlow, pyTorch, OpenCV
Languages: English, Spanish

Experience

Texas A&M University **Aug. 2019 – Aug. 2024**
Research Assistant *College Station, Texas*

- Applied data analysis and machine learning methods such as feature engineering, classification, regression, validation, and optimization to experimental, literature compiled, and simulated materials design space.
- Generated a high-throughput DFT database generator framework for different configuration structures in an alloy system. Trained a Graph Neural Network (GNN) regression model for the application of commonly expensive DFT tasks.
- Part of a computational-experimental multidisciplinary effort to design Shape Memory Alloy through hysteresis optimization via Active Learning in a Batch Bayesian Optimization based framework.
- Leveraged the CALPHAD method to generate millions of data points in a parallel high-throughput manner. Fitted to 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.

- Developed DFT automation methodologies for elastic and stability analysis in high dimensional alloy spaces.

Texas A&M University **Aug. 2022 – May 2024**
Teaching Assistant *College Station, Texas*

- **Fall 2022 Thermodynamics in Materials Science · Graduate level**
- **Spring 2023 and Spring 2024 Thermodynamics of Materials · Undergraduate level**
- Taught Thermodynamics at both the graduate and undergraduate levels, where I developed innovative problems and interactive lessons. These contributions are designed to benefit future generations at Texas A&M after I graduate.
- Created a Thermo-Calc walkthrough 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., Sauceda, 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.**, Sauceda, D., and Arroyave, R., Orlando, Florida, **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., Anaheim, California, **Feb. 2022**

Honors & Awards

Datathon 2023 Texas A&M University Major League Hacking DATATHON 2023, 2nd place in Computer Vision Challenge **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

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 2021 **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**