

GUILLERMO VAZQUEZ

PhD Candidate · Computational Material Scientist

College Station, TX

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Education

Texas A&M University

PhD in Materials Science & Engineering

Aug. 2019 – Graduation Date: May 2024

College Station, TX

Autonomous University of Queretaro

B.S. Nanotechnology Engineering

Aug. 2013 – Aug 2018

Queretaro, Mexico

Experience

Texas A&M University

Research Assistant

Aug. 2019 – May 2024

College Station, Texas

- Calculated a stiffness constant database from DFT calculations. Then a state-of-the-art ML model was engineered to act as surrogate model.
- Using the CALPHAD method we calculate in a high-throughput manner thousands of datapoints. We then fit a DNN regressor of custom architecture and use it as a kernel in optimization tasks for Material Design.
- High-Throughput generation of a DFT database for different configuration structures for an alloy system. Then a GNN regression model is trained for the application of otherwise commonly expensive DFT tasks.

Texas A&M University

Teaching Assistant

Aug. 2022 – May 2023

College Station, Texas

- **Fall 2022 Thermodynamics in Materials Science · Graduate level**
- **Spring 2023 Thermodynamics of Materials · Undergraduate level**
- 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.

Selected Publications

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.

Technical Skills

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

Framework/OSs: GitHub, Windows, Linux, MacOS

py Scientific Software: VASP, QuantumEspresso, VESTA, Xcrysden, Thermo-Calc, Origin, Gnuplot, Pandas, scikit-learn, pyTorch, TensorFlow, OpenCV

Languages: English, Spanish

Honors & Awards

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**

Youth of Excellence Prestigious Scholarship awarded to the brightest students in their undergrad class. **Sep. 2015**

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 Texas A&M University 2020 **Jun. 2020**