Guillermo Vazquez

Ph.D. Candidate · Computational Material Scientist
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Summary

- 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.).
- 7+ years of experience on Density Functional Theory (DFT).
- 5+ years of experience of Materials Design from materials simulations and data analytics.
- Fast growing author in academia with 100+ citations in 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 **Aug. 2019 – Graduation Date: May 2024**
Ph.D. in Materials Science & Engineering *College Station, TX*

Autonomous University of Queretaro **Aug. 2013 – Aug 2018**
B.S. Nanotechnology Engineering *Queretaro, Mexico*

Experience

Texas A&M University **Aug. 2019 – May 2024**
Research Assistant *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 **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**

- Created a Thermo-Calc walk-through designed for undergrad engineering students.
- Created and graded challenging and comprehensive homework sets that helped the student approach thermodynamics from a Materials Science point of view.

Selected Publications

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

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**

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**

Technical Skills

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

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**
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	**Jun. 2020**