Guillermo Vazquez

Ph.D. · Computational Material Scientist
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Enthusiast Computational scientistist with 8+ years of experience in materials design. Primary interests 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

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.
- 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.
- 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.
- **Machine Learning analytical model** (Sure Independent Screening and Sparsifying Operator) Machine Learning analytical model extrapolated from DFT calculated elastic constants.

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

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**
- **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., 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. *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**