Daniel Ocampo

J. Mike Walker '66
Department of Mechanical Engineering
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Mechanical Engineering PhD candidate at Texas A&M University. Trailblazers in Engineering fellow from Purdue University. Member of the Multiscale Mechanics of Materials Laboratory. My doctoral research is two fold: *a)* development of open-source computational codes to accelerate Density Functional Theory (DFT) calculations using machine learning; and *b)* atomistic modeling of mechanical, thermodynamical and structural properties of low-dimensional materials, including transition metal dichalcogenides (TMDs) and high entropy MXenes. Interests: computational materials science; structural and functional properties of materials; materials discovery and design.

EDUCATION

PhD in Mechanical Engineering Jan/2021-Dec/2025(exp)

Texas A&M — The University of Texas at San Antonio

Thesis advisor: Dr. Wei Gao. GPA: 3.7/4.0.

Dissertation: A Robust Methodology for Training Machine Learning Potentials from Density Functional Theory Calculations: Predicting Mechanical, Thermal, and Structural Behavior of Low-Dimensional Materials.

BS Mechanical Engineering 2014-2018

Universidad EAFIT, Medellin, Colombia

RESEARCH HISTORY

Graduate Research Assistant 2021-Present

Multiscale Mechanics of Materials Laboratory, Texas A&M University

- Stress Modulated Phase Transition in 2D Transition Metal Dichalcogenides (TMDC) Materials, $326,162.00, **Aug. 2019 - Present**, National Science Foundation (NSF) Grant 2308163.
  - Research and development of open-source code AtomDNN to train machine learning potentials from *ab-initio* Density Functional Theory (DFT) calculations.
  - High fidelity atomistic modeling of solid-solid phase transitions, dislocation-interface interactions, and the role of defects (i.e. vacancies, interstitials, etc.) in stress-induced phase transitions. PhD Wei Gao *email:*wei.gao@utsa.edu

Graduate Research Assistant 2021-Present

Multiscale Mechanics of Materials Laboratory, Texas A&M University

- CAREER: Atomistic Investigation of Phase Transition in Nanostructured Silicon–Towards Convergent Understanding with Mechanics-Informed Machine Learning Potential, $500,723.00, **October, 2021 - Present**, National Science Foundation (NSF) Grant 2305529.

- Nudge Elastic Band simulations: Set up and run simulations to find the minimum energy path and activation barriers of kink pair formation along screw dislocations.
- Theoretical Analysis: Analyze dislocation mechanics to quantify the impact of periodic boundary conditions and cell size on activation barriers.
- Validate results by comparing NEB simulations with theoretical predictions and existing data from DFT and other models.
  PhD Wei Gao *email:*wei.gao@utsa.edu

Graduate Research Assistant 2019-2020

Computational Reliability Laboratory, The University of Texas at San Antonio

- Probabilistic Modeling of Random Variables and K-Solution Developments for General Aviation – Extensions to the SMART—DT Software SmartDT website, $1,080,000, **Sep. 2016 - Dec. 2020.**, Federal Aviation Administration, FAA Grant 16-G-005.
  - Research of probabilistic methods in application to damage tolerance structures: Fracture mechanics, spectrum loading, random variable definitions, probability distributions, limit load and residual strength.
  - Calculation of single flight probability-of-failure, probability of detection curves, as well as inspection and repair methods. Numerical methods Monte Carlo sampling and First/Second Order Reliability Methods.
    PhD Harry Millwater *email:*Harry.Millwater@utsa.edu

Research Assistant 2017

EAFIT University, Medellin, Colombia

- Research and development of Indoor Positioning System (IPS) sensor, based on ultrasonic waves and its corresponding Trilateration algorithm. Research, experimentation and code development for Arduino and Matlab serial communication.
  PhD Davinson Castaño Cano *email:* dcasta25@eafit.edu.co

Research Assistant 2016-2017

Research Group of Engineering Materials, EAFIT University, Medellin, Colombia

- Code development for characterizing bone-based materials through Atomic Force Microscopy (AFM). 3D modeling and running FEM simulations.
  Ph.D Alexander Ossa H. *email:* eossa@eafit.edu.co

WORK EXPERIENCE

Graduate Teaching Assistant 2022-Present

Course: Machine learning for Mechanical engineers. Texas A&M University

- Grading, lecturing, and evaluating.
- Conferencing with students individually or in small groups.
  PhD. Wei Gao *email:* wei.gao@tamu.edu

Graduate Teaching Assistant 2020-2022

Course: Materials Engineering Laboratory. University of Texas at San Antonio UTSA

- Grading, lecturing and evaluating.
- Conducting experiments and laboratory tests, including hardness testing, tensile testing, impact testing and heat treatments.
  PhD. Madhavrao Govindaraju *email:* madhavrao.govindaraju@utsa.edu
  PhD. Alifer Crom *email:* alifer.crom@utsa.edu

Software Development Intern Spring 2018
Computational Reliability Laboratory, Dr. Harry Millwater, The University of Texas at San Antonio

- Development of Visualization Software for Aircraft Probabilistic Damage Tolerance Analysis SmartPlot: Visualization Tool for Aircraft Probabilistic Damage Tolerance Analysis.
  Harry Millwater *email:* Harry.Millwater@utsa.edu

AWARDS AND HONORS

Fellowship - Trailblazers in Engineering 2024
Purdue University, West Lafayette, IN

Fellowship - Computational Materials Science Summer School 2023
Department of Materials Science & Engineering, Texas A&M University, College Station, TX

Graduate School Competitive Research Scholarship 2020
University of Texas at San Antonio UTSA, San Antonio, TX

Visiting Scholar Grant - 1 semester research internship at UTSA 2018
University of Texas at San Antonio UTSA, San Antonio, TX

PEER-REVIEWED JOURNAL PUBLICATIONS

1. **Daniel Ocampo**, Daniela D. Posso, Reza Namakian, Wei Gao, "Adaptive Loss Weighting for Machine Learning Interatomic Potentials", *Computational Materials Science*, 2024, https://doi.org/10.1016/j.commatsci.2024.113155.

2. **Daniel Ocampo**, Reza Namakian, Chengling Wu, Fei Shuang, Wei Gao, "Unraveling the Strengthening Mechanisms and Ductility of MoVTiCrC 2D High Entropy MXenes", *npj Computational Materials*. Under preparation.

3. **Daniel Ocampo**, Fei Shuang, Reza Namakian, Wei Gao, "Machine Learning Investigation of Mirror Twin Boundary Formation in two dimensional (2D) MoTe2: Structure and Kinetics", *Computational Materials Science*. Under preparation.

4. **Daniel Ocampo**, H.R. Millwater, "SmartPlot: Visualization Tool for Aircraft Probabilistic Damage Tolerance Analysis", *UTSA Undergraduate Research and Scholarly Works*, 2018, https://hdl.handle.net/20.500.12588/67.

CONFERENCE & POSTER PRESENTATIONS

1. **Daniel Ocampo**, Daniela Posso, Reza Namakian, Wei Gao. Adaptive Loss Weighting for Machine Learning Interatomic Potentials, 2024 Materials Research Society (MRS) Spring Meeting & Exhibit, Seattle, WA.

2. Haoxuan Mu, Wei Zhang, **Daniel Ocampo**, Wei Gao, Wei Chen. Rethinking Generative Inverse Design: A Light-Weight Machine Learning Framework for On-Demand Nonlinear Materials Design, ASME 2024 International Design Engineering Technical Conferences &

Computers and Information in Engineering Conference (IDETC/CIE2024), JW Marriott, Washington, DC.

3. **Daniel Ocampo**, Wei Gao. AtomDNN: A Machine Learning Package for Atomistic Simulations, Third International Conference on Mechanics of Advanced Materials and Structures (ICMAMS), Texas A&M University, College Station, TX, 2023.

COMPUTER SKILLS

- Excellent command of Bash scripting and high performance computing (HPC) environments. Excellent command of AI and Machine learning packages Tensorflow, PyTorch. Excellent command of molecular dynamics (MD) package LAMMPS and ab-initio calculations package VASP. Knowledge of Semiconductor Physics. Experience with Bayesian Statistics and Uncertainty Quantification (UQ). Excellent command of software development tools: Git, Java, SourceTree. Excellent command of Object Oriented Programming Languages: Python, R, Matlab, C++. Excellent command of LaTeX and Microsoft Office™ tools. Excellent command of CAD software as ABAQUS and SolidWorks. Good command in FORTRAN.

ADDITIONAL COURSES

Summer Institute on High Performance Computing 2019
University of Texas at San Antonio, UTSA

- Parallel programming in C on HPC environments, GPU Accelerated Computing with C.

REFERENCES

Ph.D. Wei Gao
Associate Professor
Texas A&M University
wei.gao@tamu.com

Ph.D. Harry R. Millwater
Samuel G. Dawson Endowed Professor
University of Texas at San Antonio UTSA
harry.millwater@utsa.edu

Ph.D. Reza Namakian
Postdoctoral Researcher
Department of Mechanical Engineering - Texas A&M University
rnamak@tamu.edu

Ph.D. Çağatay Yelkarası
Research Scientist
Department of Mechanical Engineering - Texas A&M University
yelkarasi@tamu.edu