Austin Rodriguez

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SUMMARY

Ph.D. candidate in Chemical Engineering developing AI/ML methods for chemistry and materials science. Experience spans machine-learning interatomic potentials, large ab initio datasets, PyTorch framework development, distributed GPU training, periodic and molecular DFT, and molecular dynamics for battery and electrolyte systems. Interested in ML/AI roles involving scientific machine learning, force fields, molecular simulation, and data-driven materials discovery.

EDUCATION

Doctor of Philosophy in Chemical Engineering, Michigan State University, East Lansing, MI

Advisor: Jose L. Mendoza-Cortes Expected Graduation Date: **August 2026**

Proposed Dissertation Title: *Integrating Machine Learning and Density Functional Theory to Unravel and Optimize Catalytic Reaction Mechanisms*

Bachelor of Science in Chemical-Materials Engineering, Florida State University, Tallahassee, FL

GPA: 3.74 / 4.0 (Magna Cum Laude) Graduation Date: **May 2020**

EXPERIENCE

Graduate Student, Los Alamos National Laboratory, Los Alamos, NM. *May 2025 – September 2025*

- Designed and implemented Hessian-aware training pipelines for MLIPs, leveraging curvature information to improve model extrapolation, numerical stability, and molecular dynamics fidelity, reducing validation error by ~10–38% on reactive benchmarks
- Developed state-of-the-art training methods based on Hessian-vector products (HVPs) to incorporate second-order information into deep learning models, cutting training costs by ~24× compared to full Hessian approaches
- Extended the HIPPYNN PyTorch framework with custom Hessian and HVP computation nodes as well as curvature-aware loss functions, enabling scalable higher-order training across large datasets of molecular structures
- Applied my curated quantum-chemical datasets (~12,000 reactions, ~132,000 geometries) to rigorously evaluate model accuracy, generalization, and robustness on reactive potential energy surfaces
- Leveraged High Performance Computing (HPC) resources to train ML algorithms using distributed multi-node CPU/GPU training workflows to accelerate experimentation cycles

Graduate Research Assistant, Michigan State University, East Lansing, MI. *August 2021 – Present*

- Developed a deep learning interatomic potential using Density Functional Theory (DFT) energies, forces, and curvature information to accurately model molecular configurations with improved extrapolation and molecular dynamics stability at a significantly reduced computational cost than traditional methods.
- Developed a database of small organic molecules involved in approximately 68,000 chemical reactions made up of reactant, product, and transition state optimized geometries and including configurational energies, atomic forces, and Hessian matrices from Density Functional Theory calculations
- Performed DFT calculations and molecular dynamics simulations on catalytic and energy materials systems, including CO_2 reduction, CO_2 copolymerization with epoxides, oxygen evolution, Li^+FSI^--based electrolytes, and graphite intercalation in dual-ion batteries, to understand reaction mechanisms, interfacial behavior, and structure–property relationships relevant to sustainable materials design.
- Developed scalable HPC workflows for DFT, molecular dynamics, and machine-learning-enabled simulations across battery materials, catalytic reactions, and reactive molecular systems, supporting efficient computation, post-processing, and dataset generation for downstream modeling and analysis

Research Assistant, High-Performance Materials Institute (HPMI), Tallahassee, FL. *August 2019 – May 2020*

- Conducted DFT-based quantum chemical simulations to study CO_2–epoxide polymerization mechanisms and screen catalysts for improved CO_2 utilization efficiency in sustainable polymer production.

Undergraduate Researcher, Center for Advanced Power Systems (CAPS), Tallahassee, FL. *Summer 2019*

- Designed 3D SolidWorks models of gas-insulated transmission lines to analyze electric-field behavior under environmentally friendlier insulating gases.

PUBLICATIONS AND OPEN RESOURCES

Austin Rodriguez, Justin Smith, Jose L. Mendoza-Cortes, Nicholas Lubbers, Sakib Matin, Kipton Barros, "*Projected Hessian Learning: Fast Curvature Supervision for Accurate Machine-Learning Interatomic Potentials*" **Published**

Austin Rodriguez, Justin Smith, Jose L. Mendoza-Cortes, "*Does Hessian Data Improve the Performance of Machine Learning Potentials?*" **Published**

Niloofar Safaie, Austin Rodriguez, Gourhari Jana, Jose L. Mendoza-Cortes, Robert C. Ferrier, Jr., "*Unveiling the mechanisms of epoxide polymerization with N–Al adduct catalysts: a comprehensive experimental and theoretical investigation*" **Published**

Code repository: Projected Hessian Learning — *Efficient Hessian-vector-product–based training for MLIPs*

Code repository: MLFFwithHessians — *PyTorch-based Hessian-training framework for ANI-style MLIPs*

Public dataset: OpenREACT-CHON-EFH — *Quantum-chemical database of reactants, products, transition states, IRC trajectories, and NMS data*

AWARDS

SCM Research Excellence Award for Outstanding Poster Presentation at the MLCM-25 Conference — Summer 2025
Rising Star and Best Poster Abstract Award for the MLCM-25 Conference — Summer 2025
Fellowship from the Department of Chemical Engineering & Materials Science at MSU — Fall 2022
FSU's IDEA Grant Recipient — Spring 2019

SKILLS

- Proficient in programming languages such as Python, MATLAB, and Bash (Linux Shell)
- Experienced in using scientific software such as Gaussian16, Q-Chem, Material Studio and COMSOL
- Experienced with technical computing packages such as PyTorch, Scikit-learn, TensorFlow, ASE, Git, GitHub, Jupyter Notebooks, and VS Code
- Strong analytical and problem-solving skills, with experience integrating first-principles simulations, machine learning, and high-performance computing for large-scale scientific modeling.
- Demonstrated effective communication skills, including the ability to present and communicate complex concepts and ideas in English and Spanish

CONFERENCE PRESENTATIONS

- Machine Learning in Chemical and Materials Sciences 2025, Santa Fe, NM — Presented work on Hessian-trained machine learning interatomic potentials (MLIPs) for improved extrapolation and stability in reactive simulations.
- 33rd International Materials Research Congress (2025), Cancún, Mexico — Presented research integrating quantum chemistry and machine learning for materials and catalytic applications.

INVOLVEMENT

Member of Comunidad Latinoamericana (CLA) at MSU — Spring 2022 – Present
Treasurer of the Society of Petroleum Engineers — Fall 2019 – Spring 2020
Member of the Oscar Arias Sanchez Hispanic Honor Society — Fall 2019 – Spring 2020
Member of the Society of Petroleum Engineers — Fall 2018 – Spring 2021
Member of the American Institute of Chemical Engineers — Fall 2018 – Present