Ryan Morelock, Ph.D.

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Education

University of Colorado Boulder Boulder, CO
Doctor of Philosophy in Chemical Engineering August 2023
Master's in Chemical Engineering August 2021
GPA: 3.938/4.000

The University of Alabama Tuscaloosa, AL
Bachelor of Science in Chemical Engineering, Minor in Mathematics May 2018
University Honors, Chemical and Biological Engineering Departmental Honors
GPA: 4.000/4.000

Academic Honors

GAANN Fellow, University of Colorado Boulder 2019 – 2022
NSF Graduate Research Fellowship Program Honorable Mention 2020
ChBE PhD Fellowship Recipient ($10,000), University of Colorado Boulder 2018
UA Alumni Outstanding Senior Award, University of Alabama 2018
Presidential Scholarship (four years full-tuition, $2,000 research stipend), University of Alabama 2013 – 2018
Engineering Scholarship ($10,000), University of Alabama 2013 – 2018
National Merit Finalist ($2,500) 2013

Research Experience

Oak Ridge National Laboratory April 2024 – Present
Postdoctoral Researcher at the Center for Nanophase Materials Science

- Developed the python package *Ensemble-FF-fit* to dynamically parse Density Functional Theory, DFT, training data for reactive and ML force field fitting.
- Used the plane-wave based VASP code to create a DFT dataset and fit a ReaxFF reactive force field potential. This force field predicts Bi-Se bulk recrystallization during melt/quench molecular dynamics runs, in agreement with experimental observations.
- Investigated the influence of twist angle on Bi-Se/Nb 2D heterostructure topological superconductivity properties using plane-wave and real-space DFT.

University of Colorado Boulder August 2023 – April 2024
Computational Materials Science Postdoctoral Researcher

- Showed that computationally inexpensive orthorhombic surrogate structures of inorganic halide perovskites, which have applications in photovoltaics, reliably estimate the properties of much more expensive polymorphous network representations.
- Benchmarked an ~$O(10^2)$ improvement in DFT optimization times for these surrogates using VASP, to be used in high-throughput investigations of bulk crystalline halide perovskite materials. Findings submitted to The Journal of Physical Chemistry.

University of Colorado Boulder August 2018 – August 2023
Computational Materials Science GRA in Chemical Engineering

- Generated the largest database of DFT-optimized multinary perovskite oxides to date, with over 65,000 theoretical $AA'BB'O_6$ compositions characterized. Reported in Nature Scientific Data, doi:10.1038/s41597-023-02127-w.
- Used DFT to justify mixed Mn/Ni perovskite oxides' novel solar thermochemical hydrogen (STCH) production capacities in the presence of excess hydrogen. Reported in Chemistry of Materials, doi:10.1021/acs.chemmater.3c02807.

The University of Alabama January 2016 – May 2018

Undergraduate Research Assistant in Electrodeposition

- Published a new method to form the $Pd_{50}Zn_{50}$ bimetallic compound in the Journal of Electroanalytical Chemistry, doi:10.1016/j.jelechem.2018.03.003.

Georgia State University May 2015 – July 2015

Molecular Basis of Disease Undergraduate Fellow

- Quantified the abilities of zinc oxide (ZnO) nanoparticles synthesized by different pathways to inhibit Baboon lymphocryptovirus replication and propagation *in vitro*.

Research Skills

- 6+ years using DFT software packages like VASP and RMG to generate *ab initio* data.
- 6+ years of writing Python code for academic research.
    - Actively developing *Ensemble-FF-fit* for MD and ML force field fitting.
    - Developed *crystal_motifs*, a Python package that describes periodic coordination environments in crystalline solids using graph networks. This package was published in doi:10.1038/s41597-023-02127-w.
    - Developed *pparBVM*, which parallelizes our constrained bond valence parameterization procedure to capture DFT energy relationships. Published in the Journal of Chemical Theory and Computation, doi:10.1021/acs.jctc.1c01113.
- 6+ years of installing environments and debugging and compiling software on national laboratory high-performance computing platforms like NREL's Eagle and Kestrel, ORNL's Baseline, Summit and Frontier, and NERSC's Perlmutter.
- Fitting ML (GAP) and physics-based (ReaxFF) FF models for inorganic materials.

Selected Publications

- Morelock, R. J. Tran, J. T. Bare, Z. J. Trindell, J. A. McDaniel, A. H. Weimer, A. W. Musgrave, C. B. "Computationally Guided Discovery of Mixed Mn/Ni Perovskites for Solar Thermochemical Hydrogen Production at High H_2 Conversion", Chem. Mater. 2024, 36, 11, 5331–5342.
- Bare, Z. J. Morelock, R. J. Musgrave, C. B. "Dataset of theoretical multinary perovskite oxides", Sci Data, 2023, 10, 1, 244.
- Bare, Z. J. Morelock, R. J. Musgrave, C. B. "A computational framework to accelerate the discovery of perovskites for solar thermochemical hydrogen production; Identification of Gd perovskite oxide redox mediators", Advanced Functional Materials, 2022, 32.
- Morelock, R. J. Bare, Z. J. Musgrave, C. B. "Bond valence parameterization for the accurate description of DFT energetics." Journal of Chemical Theory and Computation, 2022, 18, 3257–3267.

- Park, J. E. Bare, Z. J. Morelock, R. J. Rodriguez, M. A. Ambrosini, A. Musgrave, C. B. McDaniel, A. H. Coker, E. N. "Computationally Accelerated Discovery and Experimental Demonstration of $Gd_{0.5}La_{0.5}Co_{0.5}Fe_{0.5}O_3$ for Solar Thermochemical Hydrogen Production", Frontiers in Energy Research, 2021, 9, 675.
- Xian, P. R. Morelock, R. J. Hadar, I. Musgrave, C. B. Sutton, C. "From structure mining to unsupervised exploration of atomic octahedral networks", arXiv preprint, 2023.
- Yew, S. Morelock, R. J. Musgrave, C. B. "A High-Throughput Surrogate to Polymorphous Networks for Inorganic Halide Perovskites", J. Phys. Chem., submitted.

Service and Involvement

Volunteer East Tennessee April 2024 – Present

Outdoor Cleanup and Reconstruction Volunteer

- Weeded flower beds at SEEED's (Socially Equal Energy Efficient Development) East Knoxville location, and the nature garden at Seven Islands State Birding Park (Knox County) during their Wild Yards Garden volunteer day.
- Helped rebuild the washed-out Orchard Lane section of the North Ridge Trail.
- Removed garbage from the East Fork Poplar creek (Oak Ridge) and French Broad River.

Graduate Assistance in Areas of National Need (GAANN) August 2019 – December 2022

Tutor and Leadership Committee Member

- Tutored undergraduate thermodynamics students for the Fall 2020, 2021 and 2022 semesters, and math and chemistry during Fall 2019's finals week.
- Co-led annual GAANN retreats at the YMCA of the Rockies in 2020 (Snow Mountain Ranch) and 2022 (Estes Park). Responsibilities included reserving lodging, planning daily activities and scheduling academic and industry speakers.
- Organized a panel of industry and national lab employees during the Fall 2021 semester, with representatives from NREL and Google.

Boulder's Reynolds Public Library System May 2019 – July 2019

Summer of Discovery Volunteer

- Worked with children and teens as they recorded how much they read to receive prizes and participated in scheduled activities at Boulder Public Library locations.
- Volunteered for activities including supervising a chemistry show and ushering for a library play.