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# Lane E. Schultz

## Research Assistant

Website: leschultz.github.io
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Extensive experience in workflow automation through Python, atomistic modeling, and material property predictions through machine learning techniques.

### **EDUCATION**

**Ph.D. Materials Science and Engineering**, *University of Wisconsin-Madison* (GPA: 3.691 out of 4.0) Aug 2024 **M.S. Materials Science and Engineering**, *University of Wisconsin-Madison* (GPA: 3.691 out of 4.0) Dec 2020 **B.S. Engineering**, *Fort Lewis College* (GPA: 3.99 out of 4.0)

#### SKILLS

Computational Python, Bash, Git, LTFX, C++, Verilog, MATLAB, VASP, LAMMPS, AutoCAD,

SolidWorks, Vim, Docker, Apptainer, Linux

**Quantitative Research** Workflow Automation, Atomic Modeling, Machine Learning,

Cluster Administration (OpenHPC)

**Communication** English and Spanish (fluent written and verbal)

## **TECHNICAL EXPERIENCE**

Research Assistant Jun 2018 — Present

Computational Materials Group, UW-Madison

## **Quantifying Metallic Glass Forming Ability**

- Generated ab-initio energies and forces for metallic systems to machine learn interatomic potentials

 Conducted classical, ab-initio, and machine learned molecular dynamics to model metal alloy properties and their effect on predicting glass forming ability

## **Machine Learning Domain of Applicability for Materials**

- Implemented machine learning ensemble and bagging methods for uncertainty quantification and calibration of material data sets
- Quantified model feature space dissimilarity and the effects on predicting uncertainty

## **Scientific Cluster Construction and Administration**

- Assisted in the construction and administration of two clusters
- Employed OpenHPC with Warewulf provisioning and OpenPBS queue management
  - \* 35 node machine with a total of 600 cores
  - \* 49 node machine with a total of 588 cores

## **Summer Undergraduate Research Experience**

Computational Nuclear Engineering Research Group, UW-Madison

May 2017 — Aug 2017

Madison, WI

Durango, CO

Madison, WI

- Presented "Tools for Standard Visualization of DAGMC Radiation Transport Results"
- Implemented command line tool for standard, automated image generation from data

#### **Capstone Design Project**

Sep 2016 — Apr 2017

Undergraduate Research, Fort Lewis College

Published to the American Institute of Aeronautics and Astronautics

- Designed and built an exotic propulsion test stand with a team of 5 engineering students
- Implemented electrostatic displacement mechanism and modeled system response with MATLAB

## Summer Undergraduate Research Fellowship

May 2016 — Aug 2016

Advanced Diagnostics and Propulsion Research Laboratory, Purdue

Durango, CO

- Presented "Optimization of a High-Speed X-Ray Imaging System for Studying Sprays"
- Operated pressure vessels, X-ray tube sources, and high-speed cameras for analysis of two dimensional sprays
- Built lead housing for X-ray tube sources

Dec 2015 — Apr 2016

Undergraduate Research, Fort Lewis College

Durango, CO

- Published to OCEANS 16
- Designed and developed an interchangeable sensor package for measurement of water temperature, oxygen reduction potential, pH, time, and global positioning system data

## **TEACHING EXPERIENCE**

Assisting lab peers with software installation and cluster usage
Assisted in molecular dynamic labs
Grader for Thermodynamics of Solids
Teaching Assistant for Thermal and Fluid Systems Laboratory
Teaching Assistant Engineering Fundamentals II (MATLAB)

Graduate Graduate Graduate Undergraduate Undergraduate

#### **PRESENTATIONS**

- Molecular Dynamic Characteristic Temperatures for Predicting Metallic Glass Forming Ability, 2021 Materials Science & Technology, Columbus, OH
- Molecular Dynamics Features for Predicting Metallic Glass Critical Casting Thickness, 2020 Virtual Materials Research Society Spring/Fall Meeting & Exhibit, virtual
- Design of torsional test stand for micro-newton force detection, American Institute of Aeronautics and Astronautics 2018 Conference, Atlanta, GA
- Development of a portable water quality sensor for river monitoring from small rafts, OCEANS 2016 MTS/IEEE Conference, Monterey, CA

## AWARDS, HONORS, AND SOCIETIES

- PPG Fellowship. University of Wisconsin-Madison, Madison, WI
- Ying Yu Chuang Graduate Support Award. University of Wisconsin-Madison, Madison, WI
- Sigma Pi Sigma (Physics Honor Society). Fort Lewis College, Durango, CO
- Order of the Engineer. Fort Lewis College, Durango, CO
- Deans' Council Freshman 4.0 Award and Certificate. Fort Lewis College, Durango, CO
- Freshman Chemistry Recognition Award. Fort Lewis College, Durango, CO
- Renaissance Plaque. Albuquerque, Manzano High School, NM
- Chickasaw Honor Club Outstanding Academic Achievement Award. Menard High School, Menard, TX
- Patrick S. Gilmore Band Award. Menard High School, Menard, TX

#### **PUBLICATIONS**

- L. E. Schultz, B. Afflerbach, D. Morgan, *Machine Learning Metallic Glass Critical Cooling Rates Through Atomistic and Molecular Dynamic Material Properties*, Pending publication
- L. E. Schultz, Y. Wang, R. Jacobs, D. Morgan, *Assessing Machine Learning Model Domains using Kernel Density Estimates*, Pending publication
- R. Jacobs et al., *Machine Learning Materials Properties with Accurate Predictions, Uncertainty Estimates, Domain Guidance, and Persistent Online Accessibility*, Pending Publication
- V. Agrawal et al., Accelerating Ensemble Error Bar Prediction with Single Model Fits, Computational Materials Science, Pending Publication
- J. Meng et al., *Ultra-fast oxygen conduction through vacancy-mediated mechanism in Sillén Oxychlorides*, Pending Publication
- S. Huang et al., Composition-Resolved Dynamics in Metallic Supercooled Liquids from Momentum-Resolved Electron Correlation Microscopy, Pending Publication
- B. Afflerbach et al., *Machine Learning Prediction of the Critical Cooling Rate for Metallic Glasses from Expanded Datasets and Elemental Features*, Chemistry of Materials, March 2022, DOI: 10.1021/acs.chemmater.1c03542
- L. E. Schultz, B. Afflerbach, D. Morgan, I. Szlufarska, *Molecular Dynamics Characteristic Temperatures for Predicting Metallic Glass Forming Ability*, Computational Materials Science, January 2022, DOI: 10.1016/j.commatsci.2021.110877
- L. E. Schultz, B. Afflerbach, C. Francis, D. Morgan, I. Szlufarska, P. Voyles, Exploration of Characteristic Temperature Contributions to Metallic Glass Forming Ability, Computational Materials Science, August 2021, DOI: 10.1016/j.commatsci.2021.110494
- B. Afflerbach et al., Molecular simulation-derived features for machine learning predictions of metal glass forming ability, Computational Materials Science, November 2021, DOI: 10.1016/j.commatsci.2021.110728
- J. Xi et al., Microalloying effect in ternary Al-Sm-X (X = Ag, Au, Cu) metallic glasses studied by ab initio molecular dynamics, Computational Materials Science, December 2020, DOI: 10.1016/j.commatsci.2020.109958
- L. E. Schultz, T. J. Cogger, J. Schneider, R. Good, R. Rothschild, and W. Nollet, *Design of torsional test stand for micro-newton force detection*, Aerodynamic Measurement Technology and Ground Testing Conference, June 2018, DOI: 10.2514/6.2018-3737
- J. Schneider, L. E. Schultz, S. Mancha, E. Hicks, and R. N. Smith, *Development of a portable water quality sensor for river monitoring from small rafts*, OCEANS 2016 MTS/IEEE Monterey, September 2016, DOI: 10.1109/OCEANS.2016.7761392

#### **INTERESTS**

Movies, shows, video games, weight lifting, LEGOs, PC building, and coding