(806) 678-6904
Madison, WI
lsschultz@wisc.edu

Lane E. Schultz

Research Assistant

Website: leschultz.github.io
GitHub: leschultz
LinkedIn: lane-schultz-983920236

Research assistant with expertise in machine learning, cluster administration, and modeling materials, seeking to advance materials research.

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) Dec 2017

Skills

Computational	PyTorch, scikit-learn, Python, Bash, Git, LaTeX, 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 — Aug 2024**
Computational Materials Group, UW-Madison *Madison, WI*

Machine Learning Domain of Applicability for Materials

- Implemented machine learning model ensemble for property prediction and uncertainty quantification of material data
- Quantified the feature space of the model using kernel density estimation to identify regions where the model's predictions were less accurate.
- Wrote PyPI package for users to apply machine learning models that flag improper predictions

Scientific Cluster Construction and Administration

- Assisted in the construction and administration of two clusters
- Employed OpenHPC with Warewulf provisioning and OpenPBS queue management
- Compiled software and used Environment Modules to setup software for materials research: VASP, LAMMPS, Python, etc.

Quantifying Metallic Glass Forming Ability

- High throughput generation of ab-initio energies and forces for metallic systems to machine learn 34 interatomic potentials
- Conducted classical, ab-initio, and machine learned molecular dynamics to model metal alloy properties and their effect on predicting glass forming ability

Summer Undergraduate Research Experience **May 2017 — Aug 2017**
Computational Nuclear Engineering Research Group, UW-Madison *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 *Durango, CO*

- **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

Design Project **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

Publications

- L. E. Schultz *et al.*, "Machine learning metallic glass critical cooling rates through atomistic and molecular dynamic material properties," Pending Publication
- L. E. Schultz *et al.*, "A general approach for determining applicability domain of machine learning models," 2024. arXiv: 2406.05143
- L. E. Schultz *et al.*, "Molecular dynamic characteristic temperatures for predicting metallic glass forming ability," *Computational Materials Science*, vol. 201, p. 110 877, 2022, ISSN: 0927-0256. DOI: https://doi.org/10.1016/j.commatsci.2021.110877. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0927025621005899
- L. E. Schultz *et al.*, "Exploration of characteristic temperature contributions to metallic glass forming ability," *Computational Materials Science*, vol. 196, p. 110 494, 2021, ISSN: 0927-0256. DOI: https://doi.org/10.1016/j.commatsci.2021.110494. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0927025621002196
- L. E. Schultz *et al.*, "Design of torsional test stand for micro-newton force detection," in *2018 Aerodynamic Measurement Technology and Ground Testing Conference*. 2018. DOI: 10.2514/6.2018-3737. [Online]. Available: https://arc.aiaa.org/doi/abs/10.2514/6.2018-3737
- J. Meng *et al.*, "Ultra-fast oxygen conduction in sillén oxychlorides," 2024. arXiv: 2406.07723
- R. Jacobs *et al.*, "Machine learning materials properties with accurate predictions, uncertainty estimates, domain guidance, and persistent online accessibility," Pending Publication
- S. Huang *et al.*, "Composition-resolved dynamics in metallic supercooled liquids from momentum-resolved electron correlation microscopy," Pending Publication
- V. Agrawal *et al.*, "Accelerating ensemble error bar prediction with single models fits," 2024. arXiv: 2404.09896
- K. Schmidt *et al.*, "Foundry-ml - software and services to simplify access to machine learning datasets in materials science," *Journal of Open Source Software*, vol. 9, no. 93, p. 5467, 2024. DOI: 10.21105/joss.05467. [Online]. Available: https://doi.org/10.21105/joss.05467
- B. T. Afflerbach *et al.*, "Machine Learning Prediction of the Critical Cooling Rate for Metallic Glasses from Expanded Datasets and Elemental Features," *Chemistry of Materials*, acs.chemmater.1c03542, Mar. 2022, ISSN: 0897-4756. DOI: 10.1021/acs.chemmater.1c03542. [Online]. Available: https://pubs.acs.org/doi/10.1021/acs.chemmater.1c03542

- B. T. Afflerbach *et al.*, "Molecular simulation-derived features for machine learning predictions of metal glass forming ability," *Computational Materials Science*, vol. 199, Nov. 2021, ISSN: 09270256. 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*, vol. 185, p. 109 958, 2020, ISSN: 0927-0256. DOI: https://doi.org/10.1016/j.commatsci.2020.109958. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0927025620304493
- B. Halls *et al.*, "Quantitative 10-50 khz x-ray radiography of liquid spray distributions using a rotating-anode tube source," *International Journal of Multiphase Flow*, vol. 109, pp. 123–130, 2018, ISSN: 0301-9322. DOI: https://doi.org/10.1016/j.ijmultiphaseflow.2018.07.014. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0301932218301198
- J. Schneider *et al.*, "Development of a portable water quality sensor for river monitoring from small rafts," in *OCEANS 2016 MTS/IEEE Monterey*, 2016, pp. 1–10. DOI: 10.1109/OCEANS.2016.7761392

Presentations

- "Molecular dynamic characteristic temperatures for predicting metallic glass forming ability," Materials Science & Technology, Columbus, OH, 2021
- "Molecular dynamics features for predicting metallic glass critical casting thickness," Virtual Materials Research Society Spring/Fall Meeting & Exhibit, Virtual, 2020
- "Design of torsional test stand for micro-newton force detection," American Institute of Aeronautics and Astronautics, Atlanta, GA, 2018
- "Development of a portable water quality sensor for river monitoring from small rafts," OCEANS, Monterey, CA, 2016

Teaching Experience

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

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

Interests

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