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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) 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 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

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

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
- 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
- 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

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

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

Interests

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