Lane E. Schultz

Research Assistant

Website: leschultz.github.io GitHub: leschultz

LinkedIn: lane-schultz-983920236

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 PyTorch, scikit-learn, Python, Bash, Git, ŁTFX, 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 materials 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

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Summer Undergraduate Research Fellowship

Advanced Diagnostics and Propulsion Research Laboratory, Purdue

May 2016 — Aug 2016 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

JOURNAL PUBLICATIONS

- L. E. Schultz, B. Afflerbach, I. Szlufarska, and D. Morgan, "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, B. Afflerbach, C. Francis, P. M. Voyles, I. Szlufarska, and D. Morgan, "Exploration of characteristic temperature contributions to metallic glass forming ability", *Computational Materials Science*, vol. 196, p. 110 494, 2021, ISSN: 0927-0256. DOI:

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https://doi.org/10.1016/j.commatsci.2021.110494.[Online]. Available: https://www.sciencedirect.com/science/article/pii/S0927025621002196
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- K. Schmidt, A. Scourtas, L. Ward, S. Wangen, M. Schwarting, I. Darling, E. Truelove, A. Ambadkar, R. Bose, Z. Katok, J. Wei, X. Li, R. Jacobs, L. Schultz, D. Kim, M. Ferris, P. M. Voyles, D. Morgan, I. Foster, and B. Blaiszik, "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, C. Francis, L. E. Schultz, J. Spethson, V. Meschke, E. Strand, L. Ward, J. H. Perepezko, D. Thoma, P. M. Voyles, I. Szlufarska, and D. Morgan, "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, L. Schultz, J. H. Perepezko, P. M. Voyles, I. Szlufarska, and D. Morgan, "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, G. Bokas, L. Schultz, M. Gao, L. Zhao, Y. Shen, J. Perepezko, D. Morgan, and I. Szlufarska, "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, J. Gord, L. Schultz, W. Slowman, M. Lightfoot, S. Roy, and T. Meyer, "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:

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https://doi.org/10.1016/j.ijmultiphaseflow.2018.07.014.[Online]. Available: https://www.sciencedirect.com/science/article/pii/S0301932218301198
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PENDING JOURNAL ACCEPTANCE

- L. E. Schultz, Y. Wang, R. Jacobs, and D. Morgan, "A general approach for determining applicability domain of machine learning models", *npj Computational Materials*, 2024. arXiv: 2406.05143
- J. Meng, M. S. Sheikh, L. E. Schultz, W. O. Nachlas, J. Liu, M. P. Polak, R. Jacobs, and D. Morgan, "Ultra-fast oxygen conduction in sillén oxychlorides", *Advanced Energy Materials*, 2024. arXiv: 2406.07723
- R. Jacobs, L. E. Schultz, A. Scourtas, K. Schmidt, O. Price, W. Engler, B. Blaiszik, and D. Morgan, "Machine learning materials properties with accurate predictions, uncertainty estimates, domain guidance, and persistent online accessibility", *npj Computational Materials*,
- V. Agrawal, S. Zhang, L. E. Schultz, and D. Morgan, "Accelerating ensemble error bar prediction with single models fits", *Computational Materials Science*, 2024. arXiv: 2404.09896

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
- L. E. Schultz, T. J. Cogger, R. Good, J. Schneider, R. Rothschild, and W. Nollet, "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. 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", 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 Graduate

Assisted in molecular dynamic labs

Graduate

• Grader for Thermodynamics of Solids

Undergraduate

Teaching Assistant for Thermal and Fluid Systems Laboratory

Undergraduate

Teaching Assistant Engineering Fundamentals II (MATLAB)

AWARDS, HONORS, AND SOCIETIES

PPG Fellowship

• Order of the Engineer

University of Wisconsin-Madison, Madison, WI

Ying Yu Chuang Graduate Support Award

University of Wisconsin-Madison, Madison, WI Fort Lewis College, Durango, CO

• Sigma Pi Sigma (Physics Honor Society)

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

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