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Lane Enrique Schultz
Curriculum Vitae

LinkedIn: lane-schultz-983920236
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GitHub: leschultz

Education

Ph.D. Materials Science and Engineering, *University of Wisconsin-Madison*	(GPA: 3.70/4.0)	Aug 2024
M.S. Materials Science and Engineering, *University of Wisconsin-Madison*	(GPA: 3.70/4.0)	Dec 2020
B.S. Engineering, *Fort Lewis College*	(GPA: 3.99/4.0)	Dec 2017

Skills

Tools	Python, PyTorch, scikit-learn, Bash, Git, LaTeX, C++, Verilog, MATLAB, OpenHPC, Vim, Docker, Apptainer, Linux, VASP, LAMMPS, AutoCAD, SolidWorks
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:** Developed a method to determine the domain of applicability for machine learning models in materials property prediction. Utilized kernel density estimation to measure dissimilarity between test and training data in feature space. This measure effectively distinguishes chemically distinct groups and correlates high dissimilarity with poor model performance and unreliable uncertainty estimates. Provided automated tools for researchers via a package on GitHub and PyPI.
- **Scientific Cluster Construction and Administration:** Assisted in building and managing two high-performance computing clusters using OpenHPC with Warewulf provisioning and OpenPBS queue management. Compiled materials research software including VASP, LAMMPS, and Python. Implemented Environment Modules to streamline software management, enhancing research efficiency and reproducibility.
- **Quantifying Metallic Glass Forming Ability:** Developed a high-throughput workflow for efficiently training machine learning interatomic potentials and simulating complex material properties. Developed predictive models for metallic glass forming ability using elemental and simulated properties. Demonstrated that key trends in properties with glass forming ability aligned with prior research insights from others.

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

- **Developed Python Tool:** Automated the visualization of Direct Accelerated Geometry Monte Carlo (DAGMC) geometries in VisIt.
- **Collaboration Friendly Code:** The Python PEP 8 coding style was adopted to facilitate easier reading.

Capstone Design Project **Sep 2016 — Apr 2017**
Undergraduate Research, Fort Lewis College . . . . . Durango, CO

- **Built Instrumentation:** Team designed and built an exotic propulsion test stand.
- **MATLAB Modeling:** Implemented electrostatic displacement mechanism and modeled system response.

Summer Undergraduate Research Fellowship **May 2016 — Aug 2016**
Advanced Diagnostics and Propulsion Research Laboratory, Purdue . . . . . Durango, CO

- **Experimental Imaging:** Operated pressure vessels, X-ray tube sources, and high-speed cameras for analysis of two dimensional sprays.
- **Lead Shielding:** Constructed a protective lead enclosure for X-ray tube sources to shield operating personnel from excessive radiation exposure.

Design Project **Dec 2015 — Apr 2016**
Undergraduate Research, Fort Lewis College . . . . . Durango, CO

- **Sensor Package:** Designed and developed an interchangeable sensor package for measurement of water temperature, oxygen reduction potential, pH, time, and global positioning system data.
- **Simple Deployment:** Package designed to be durable, waterproof, and easy to use by attaching to rafts or kayaks.

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: https://doi.org/10.1016/j.commatsci.2021.110494. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0927025621002196
- 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: https://doi.org/10.1016/j.ijmultiphaseflow.2018.07.014. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0301932218301198

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
- L. E. Schultz, B. Afflerbach, and D. Morgan, "Machine learning metallic glass critical cooling rates through elemental and molecular simulation based featurization," In Preparation
- S. Huang, A. Annamareddy, C. Francis, L. E. Schultz, J. Ketkaew, M. D. Ediger, L. Yu, J. Schroers, D. Morgan, and P. M. Voyles1, "Composition-resolved dynamics in metallic supercooled liquids from momentum-resolved electron correlation microscopy," In Preparation

Presentations

- L. Schultz, B. T. Afflerbach, and D. Morgan, "Molecular dynamic characteristic temperatures for predicting metallic glass forming ability," Materials Science & Technology, Columbus, OH, 2021
- L. Schultz, B. T. Afflerbach, and D. Morgan, "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 undergraduates with research — Undergraduate
- Assisting laboratory group peers with software installation and cluster use — 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

Professional References

Dane Morgan — Professor of Materials and Engineering (University of Wisconsin-Madison)
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Izabela Szlufarska — Professor and Chair of Materials and Engineering (University of Wisconsin-Madison)
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Paul Voyles — Professor of Materials and Engineering (University of Wisconsin-Madison)
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Additional Information

Interests — Movies, shows, video games, weight lifting, LEGOs, PC building, and coding
Citizenship — United States, Colombia, and the Chickasaw Nation