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Lane E. Schultz

Research Assistant

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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

Tools	Python, PyTorch, scikit-learn, Bash, Git, LaTeX, C++, Verilog, MATLAB, Vim, Docker, Apptainer, Linux, VASP, LAMMPS, AutoCAD, SolidWorks
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:** 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 computed elemental properties and simulated features. Demonstrated that key trends in properties with glass forming ability aligned with prior research insights.

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

- Developed a Python toolkit for automating and visualizing direct accelerated geometry monte carlo geometries in VisIt.
- The Python PEP 8 coding style was adopted to facilitate easier reading and collaboration among users.

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

- 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

- Operated pressure vessels, X-ray tube sources, and high-speed cameras for analysis of two dimensional sprays.

- 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

- 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: 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

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 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