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# Lane E. Schultz, Ph.D.

Résumé

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## Education

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|---|---|---|
| **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

Python, PyTorch, scikit-learn, Bash, Git, LaTeX, C++, OpenHPC, Vim, Docker, Apptainer, Linux, VASP, LAMMPS

## 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 using kernel density estimation to assess the applicability domain of machine learning models. The method effectively distinguishes chemically distinct groups and relates high dissimilarity with poor model performance and unreliable uncertainty estimates.
- **Scientific Cluster Construction and Administration:** Assisted in building and managing two high-performance computing clusters. Compiled materials research software and implemented Environment Modules to streamline software management.
- **Quantifying Metallic Glass Forming Ability:** Developed a high-throughput workflow for efficiently training machine learning interatomic potentials and simulating complex material properties. Properties were used to develop models for metallic glass forming ability and followed physically rational trends observed in previous research.

**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 . . . . . West Lafayette, IN

- **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

- Lane E. Schultz, Benjamin Afflerbach, Izabela Szlufarska, and Dane Morgan. "Molecular dynamic characteristic temperatures for predicting metallic glass forming ability". In: *Computational Materials Science* (2022). DOI: 10.1016/j.commatsci.2021.110877
- Lane E. Schultz, Benjamin Afflerbach, Carter Francis, Paul M. Voyles, Izabela Szlufarska, and Dane Morgan. "Exploration of characteristic temperature contributions to metallic glass forming ability". In: *Computational Materials Science* (2021). DOI: 10.1016/j.commatsci.2021.110494
- Vidit Agrawal, Shixin Zhang, Lane E. Schultz, and Dane Morgan. "Accelerating ensemble uncertainty estimates in supervised materials property regression models". In: *Computational Materials Science* (2025). DOI: 10.1016/j.commatsci.2024.113494
- Kj Schmidt, Aristana Scourtas, Logan Ward, Steve Wangen, Marcus Schwarting, Isaac Darling, Ethan Truelove, Aadit Ambadkar, Ribhav Bose, Zoa Katok, Jingrui Wei, Xiangguo Li, Ryan Jacobs, Lane Schultz, Doyeon Kim, Michael Ferris, Paul M. Voyles, Dane Morgan, Ian Foster, and Ben Blaiszik. "Foundry-ML - Software and Services to Simplify Access to Machine Learning Datasets in Materials Science". In: *Journal of Open Source Software* (2024). DOI: 10.21105/joss.05467
- Benjamin T. Afflerbach, Carter Francis, Lane E. Schultz, Janine Spethson, Vanessa Meschke, Elliot Strand, Logan Ward, John H. Perepezko, Dan Thoma, Paul M. Voyles, Izabela Szlufarska, and Dane Morgan. "Machine Learning Prediction of the Critical Cooling Rate for Metallic Glasses from Expanded Datasets and Elemental Features". In: *Chemistry of Materials* (2022). DOI: 10.1021/acs.chemmater.1c03542
- Benjamin T. Afflerbach, Lane Schultz, John H. Perepezko, Paul M. Voyles, Izabela Szlufarska, and Dane Morgan. "Molecular simulation-derived features for machine learning predictions of metal glass forming ability". In: *Computational Materials Science* (2021). DOI: 10.1016/j.commatsci.2021.110728
- J. Xi, G. Bokas, L.E. Schultz, M. Gao, L. Zhao, Y. Shen, J.H. 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". In: *Computational Materials Science* (2020). DOI: 10.1016/j.commatsci.2020.109958
- B.R. Halls, J.R. Gord, L.E. Schultz, W.C. Slowman, M.D.A. Lightfoot, S. Roy, and T.R. Meyer. "Quantitative 10-50 kHz X-ray radiography of liquid spray distributions using a rotating-anode tube source". In: *International Journal of Multiphase Flow* (2018). DOI: 10.1016/j.ijmultiphaseflow.2018.07.014

## Submitted for Publication

- Lane E. Schultz, Yiqi Wang, Ryan Jacobs, and Dane Morgan. "A General Approach for Determining Applicability Domain of Machine Learning Models". In: *npj Computational Materials* (2024). URL: https://arxiv.org/abs/2406.05143
- Jun Meng, Md Sariful Sheikh, Lane E. Schultz, William O. Nachlas, Jian Liu, Maciej P. Polak, Ryan Jacobs, and Dane Morgan. "Ultra-fast Oxygen Conduction in Sillén Oxychlorides". In: *Advanced Energy Materials* (2024). URL: https://arxiv.org/abs/2406.07723
- Ryan Jacobs, Lane E. Schultz, Aristana Scourtas, KJ Schmidt, Owen Price, Will Engler, Ben Blaiszik, and Dane Morgan. "Machine Learning Materials Properties with Accurate Predictions, Uncertainty Estimates, Domain Guidance, and Persistent Online Accessibility". In: *Machine Learning: Science and Technology* (2024). URL: https://arxiv.org/abs/2406.15650
- L. E. Schultz, B. Afflerbach, P. M. Voyles, and D. Morgan. "Machine Learning Metallic Glass Critical Cooling Rates Through Elemental and Molecular Simulation Based Featurization". In: *Journal of Materiomics* (2024)