

EDUCATION

Ph.D. Materials Science and Engineering , <i>University of Wisconsin-Madison</i> (GPA: 3.691 out of 4.0)	Aug 2024
M.S. Materials Science and Engineering , <i>University of Wisconsin-Madison</i> (GPA: 3.691 out of 4.0)	Dec 2020
B.S. Engineering , <i>Fort Lewis College</i> (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 Computational Materials Group, UW-Madison	Jun 2018 — Aug 2024 Madison, WI
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- **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 Computational Nuclear Engineering Research Group, UW-Madison	May 2017 — Aug 2017 Madison, WI
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- **Presented** "Tools for Standard Visualization of DAGMC Radiation Transport Results"
- Implemented command line tool for standard, automated image generation from data

Capstone Design Project Undergraduate Research, Fort Lewis College	Sep 2016 — Apr 2017 Durango, CO
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- **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 Advanced Diagnostics and Propulsion Research Laboratory, Purdue	May 2016 — Aug 2016 Durango, CO
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- **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

Undergraduate Research, Fort Lewis College

Dec 2015 — Apr 2016

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: <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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://arxiv.org/abs/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

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| • 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

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| • 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