

Research assistant with expertise in machine learning, cluster administration, and modeling materials, seeking to advance materials research.

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

Computational	PyTorch, scikit-learn, Python, Bash, Git, \LaTeX , 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 <i>Computational Materials Group, UW-Madison</i>	Jun 2018 — Aug 2024 <i>Madison, WI</i>
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Machine Learning Domain of Applicability for Materials

- Implemented machine learning model ensemble for property prediction and uncertainty quantification of material 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 <i>Computational Nuclear Engineering Research Group, UW-Madison</i>	May 2017 — Aug 2017 <i>Madison, WI</i>
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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 <i>Undergraduate Research, Fort Lewis College</i>	Sep 2016 — Apr 2017 <i>Durango, CO</i>
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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

May 2016 — Aug 2016

Advanced Diagnostics and Propulsion Research Laboratory, Purdue

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

PUBLICATIONS

- L. E. Schultz *et al.*, “Machine learning metallic glass critical cooling rates through atomistic and molecular dynamic material properties,” Pending Publication
- L. E. Schultz *et al.*, “A general approach for determining applicability domain of machine learning models,” 2024. arXiv: 2406.05143
- L. E. Schultz *et al.*, “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 *et al.*, “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>
- L. E. Schultz *et al.*, “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. Meng *et al.*, “Ultra-fast oxygen conduction in sillén oxychlorides,” 2024. arXiv: 2406.07723
- R. Jacobs *et al.*, “Machine learning materials properties with accurate predictions, uncertainty estimates, domain guidance, and persistent online accessibility,” Pending Publication
- S. Huang *et al.*, “Composition-resolved dynamics in metallic supercooled liquids from momentum-resolved electron correlation microscopy,” Pending Publication
- V. Agrawal *et al.*, “Accelerating ensemble error bar prediction with single models fits,” 2024. arXiv: 2404.09896
- K. Schmidt *et al.*, “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 *et al.*, “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 *et al.*, “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 *et al.*, “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 *et al.*, “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>
- J. Schneider *et al.*, “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](https://doi.org/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 |

PRESENTATIONS

- *Molecular Dynamic Characteristic Temperatures for Predicting Metallic Glass Forming Ability*, 2021 Materials Science & Technology, Columbus, OH
- *Molecular Dynamics Features for Predicting Metallic Glass Critical Casting Thickness*, 2020 Virtual Materials Research Society Spring/Fall Meeting & Exhibit, virtual
- *Design of torsional test stand for micro-newton force detection*, American Institute of Aeronautics and Astronautics 2018 Conference, Atlanta, GA
- *Development of a portable water quality sensor for river monitoring from small rafts*, OCEANS 2016 MTS/IEEE Conference, Monterey, CA

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