

Extensive experience in workflow automation through Python, atomistic modeling, and material property predictions through machine learning techniques.

EDUCATION

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| 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

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| 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

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| 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 ensemble and bagging methods for uncertainty quantification and calibration of material data sets
- Quantified model feature space dissimilarity and the effects on predicting uncertainty

Scientific Cluster Construction and Administration

- Assisted in the construction and administration of two clusters
- Employed OpenHPC with Warewulf provisioning and OpenPBS queue management
 - * 35 node machine with a total of 600 cores
 - * 49 node machine with a total of 588 cores

Quantifying Metallic Glass Forming Ability

- Generated ab-initio energies and forces for metallic systems to machine learn interatomic potentials
- Conducted classical, ab-initio, and machine learned molecular dynamics to model metal alloy properties and their effect on predicting glass forming ability

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| 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

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| 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

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| Summer Undergraduate Research Fellowship <i>Advanced Diagnostics and Propulsion Research Laboratory, Purdue</i> | May 2016 — Aug 2016 <i>Durango, CO</i> |
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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

- **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

- 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

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- *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