

Research Experience

- **Phases Research Lab, Pennsylvania State University**
NASA Space Technology Research Fellow (Advisor: Zi-Kui Liu)

 - Developed uncertainty quantification methods for CALPHAD modeling through development of pycalphad and ESPEI, open research and education software for computational thermodynamics
 - Established ICME approaches for designing functionally graded, additively manufactured materials
 - Designed methods for high-throughput first-principles DFT calculations for metals and alloys
 - Co-organized and delivered two workshops on “[Software Tools from Atomistics to Phase Diagrams](#)” with over 140 total attendees (November 10-11, 2020 and December 8-9, 2020)
 - Mentored undergraduate students in the Women In Science and Engineering Research (WISER) program

University Park, PA
2016 – Present
 - **NASA Jet Propulsion Lab**
Graduate Research Intern (Mentors: Richard Otis, Peter Dillon)

 - Used computational thermodynamics to develop bulk metallic glass alloy composition specifications
 - Developed a model for oxygen tolerance in bulk metallic glasses

La Cañada Flintridge, CA
05/2017 – 08/2017
 - **Solid State Ionics Laboratory, Michigan State University**
Undergraduate Research Assistant (Advisor: Jason D. Nicholas)

 - Fabricated and improved the performance of solid oxide fuel cells
 - Characterized fuel cells with EIS, XRD, and SEM

East Lansing, MI
2015 – 2016
 - **Composite Materials & Structures Center, Michigan State University**
Undergraduate Research Assistant (Advisor: Lawrence T. Drzal)

 - Designed a graphene nanoplatlet-based capacitive deionization cell
 - Characterized graphene nanoplatelet papers using scanning electron microscopy

East Lansing, MI
2014 – 2015
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Teaching Experience

- **Department of Materials Science and Engineering, Pennsylvania State University**
Teaching Assistant

 - (*Spring 2020*) MatSE 410: Phase Relations in Materials Systems
 - (*Spring 2018*) MatSE 404/BME 444: Surfaces and the Biological Response to Materials
 - (*Spring 2017*) MatSE 462: General Properties Laboratory in Materials

University Park, PA
2016 – Present
 - **College of Engineering, Michigan State University**
Undergraduate Lab Mentor

 - (*Spring 2016*) EGR 102: Introduction to Engineering Modeling
 - (*Fall 2015*) EGR 100: Introduction to Engineering Design
 - (*Fall 2015*) EGR 291: Spatial Visualization

East Lansing, MI
2015 – 2016
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Education

- **Pennsylvania State University**
Ph.D., Materials Science and Engineering; Graduate Minor, Computational Materials

 - 3.74 GPA
 - NASA Space Technology Research Fellow (2018 – Present)
 - NSF Research Trainee in the CoMET Program (dftcomet.psu.edu) (2016 – 2018)

University Park, PA
2016 – Present
 - **Michigan State University**
B.S. Materials Science and Engineering

 - 3.56 GPA
 - Dean’s List, 5 semesters

East Lansing, MI
2012 – 2016
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Awards and Honors

- Robert E. Newnham Award for Research Excellence, Pennsylvania State University 2020
- Larry Kaufman Scholarship, Calphad XLIX Conference 2020
- Runner Up, NASA Software of the Year (SoY) award - *pycalphad* 2019
- Honorable Mention, National Science Foundation Graduate Research Fellowship Program 2018
- Outstanding Contribution in Reviewing - *CALPHAD Journal* 2017
- Travel Award for iMATSE Graduate Students, Pennsylvania State University 2017
- Helen R. and Van H. Leichter Graduate Fellowship, Pennsylvania State University 2016
- College of Engineering Endowed Opportunity Fund scholarship, Michigan State University 2015

Publications

15. L.D. Bobbio, **B. Bocklund**, Z.-K. Liu, A.M. Beese, Tensile behavior of stainless steel 304L to Ni-20Cr functionally graded material: experimental characterization and computational simulations, *Submitted*. Preprint: [arXiv ID: 2102.00120](#).
14. C. Wang, S.-L. Shang, J. You, **B. Bocklund**, Y. Wang, H.-Y. Wang, Z.-K. Liu, Understanding the effect of oxygen on the glass-forming ability of Zr₄₃Cu₄₃Al₇Be₇ bulk metallic glass by ab initio molecular dynamics simulations *Submitted*.
13. P. Vogt, F.V.E. Hensling, K. Azizie, C.S. Chang, D. Turner, J. Park, J.P. McCandless, H. Paik, **B. Bocklund**, G. Hoffman, O. Bierwagen, D. Jena, H.G. Xing, S. Mou, D.A. Muller, S.-L. Shang, Z.-K. Liu, D.G. Schlom, Adsorption-Controlled Growth of Ga₂O₃ by Suboxide Molecular-Beam Epitaxy, *Featured APL Materials* 9(3) 031101. [doi: 10.1063/5.0035469](#).
12. R. Otis, **B. Bocklund**, Z.-K. Liu, Sensitivity estimation for calculated phase equilibria, *Journal of Materials Research* (2020) 1–11. [doi: 10.1557/jmr.2020.269](#).
11. K.M. Adkison, S.-L. Shang, **B. Bocklund**, D. Klimm, D.G. Schlom, Z.-K. Liu, Suitability of binary oxides for molecular-beam epitaxy source materials: A comprehensive thermodynamic analysis, *Featured APL Materials* 8 (2020) 081110. [doi: 10.1063/5.0013159](#).
10. S. Zomorodpoosh, **B. Bocklund**, A. Obaied, R.A. Otis, Z.-K. Liu, I. Roslyakova, Statistical approach for automated weighting of datasets: Application to heat capacity data, *CALPHAD* 71 (2020) 101994. [doi: 10.1016/j.calphad.2020.101994](#).
9. **B. Bocklund**, L.D. Bobbio, R.A. Otis, A.M. Beese, Z.-K. Liu, Scheil-Gulliver simulations for the design of functionally graded alloys by additive manufacturing using pycalphad, *Materialia* 11 (2020) 100689. [doi: 10.1016/j.mtla.2020.100689](#).
8. A. Obaied, **B. Bocklund**, S. Zomorodpoosh, L. Zhang, R. Otis, Z.-K. Liu, I. Roslyakova, Thermodynamic re-assessment of pure chromium using modified segmented regression model, *CALPHAD* 69 (2020) 101762. [doi: 10.1016/j.calphad.2020.101762](#).
7. L.D. Bobbio, **B. Bocklund**, A. Reichardt, R.A. Otis, J.P. Borgonia, R.P. Dillon, A.A. Shapiro, B.W. McEnerney, P. Hosemann, Z.-K. Liu, A.M. Beese, Analysis of formation and growth of the σ phase in additively manufactured functionally graded materials, *Journal of Alloys and Compounds* 814 (2020) 151729. [doi: 10.1016/j.jallcom.2019.151729](#).
6. **B. Bocklund**, R.A. Otis, A. Egorov, A. Obaied, I. Roslyakova, Z.-K. Liu, ESPEI for efficient thermodynamic database development, modification, and uncertainty quantification: application to Cu-Mg, *MRS Communications* 9(2) (2019) 618–627. [doi: 10.1557/mrc.2019.59](#).
5. N.H. Paulson, **B. Bocklund**, R.A. Otis, Z.-K. Liu, S. Marius, Quantified Uncertainty in Thermodynamic Modeling for Materials Design. *Acta Materialia* 174 (2019) 9–15. [doi: 10.1016/j.actamat.2019.05.017](#).
4. Y. Wang, Y.-J. Hu, **B. Bocklund**, S.-L. Shang, B.-C. Zhou, Z.-K. Liu, L.-Q. Chen, First-principles thermodynamic theory of Seebeck coefficients, *Physical Review B* 98 (2018) 224101. [doi: 10.1103/PhysRevB.98.224101](#).
3. L.D. Bobbio, **B. Bocklund**, R.A. Otis, J.P. Borgonia, R.P. Dillon, A.A. Shapiro, B. McEnerney, Z.-K. Liu, A.M. Beese, Characterization of a functionally graded material of Ti-6Al-4V to 304L stainless steel with an intermediate V section. *Journal of Alloys and Compounds* 742 (2018) 1031–1036. [doi: 10.1016/j.jallcom.2018.01.156](#)
2. L.D. Bobbio, **B. Bocklund**, R.A. Otis, J.P. Borgonia, R.P. Dillon, A.A. Shapiro, B. McEnerney, Z.-K. Liu, A.M. Beese, Experimental analysis and thermodynamic calculations of an additively manufactured functionally graded material of V to Invar 36, *Journal of Materials Research* 33 (2018) 1642–1649. [doi: 10.1557/jmr.2018.92](#).
1. K. Mathew, J.H. Montoya, A. Faghaninia, S. Dwarakanath, M. Aykol, H. Tang, I. Chu, T. Smidt, **B. Bocklund**, M. Horton, J. Dagdelen, B. Wood, Z.-K. Liu, J. Neaton, S.P. Ong, K. Persson, A. Jain, Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. *Computational Materials Science* 139, 140–152 (2017). [doi: 10.1016/j.commatsci.2017.07.030](#)

Presentations

10. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2020, February). Uncertainty quantification and propagation in ICME enabled by ESPEI. TMS 2020 Annual Meeting, San Diego, CA.
9. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2019, October) *Invited*. Automated CALPHAD modeling and uncertainty quantification of a ternary system using ESPEI. Materials Science and Technology 2019, Portland, OR.
8. **B. Bocklund**, R.A. Otis*, Z.-K. Liu (2019, June). *Software Workshop*: pycalphad and ESPEI. CALPHAD XLVIII, Singapore.
7. N.H. Paulson, **B. Bocklund***, R.A. Otis, Z.-K. Liu, M. Stan (2019, June). Quantified Uncertainty in CALPHAD for Materials Design. CALPHAD XLVIII, Singapore.
6. **B. Bocklund***, L.D. Bobbio, R.A. Otis, S. Shang, A.M. Beese, Z.-K. Liu (2019, March). Impact of Uncertainty Quantification in Automated Calphad Modeling on the design of Additively Manufactured, Functionally-graded Alloys. TMS 2019 Annual Meeting, Phoenix, AZ.
5. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2018, October). Computational Tools for the Automated Development of a Cr-Fe-Ni-Ti-V CALHPAD Database. Materials Science and Technology 2018, Columbus, OH.
4. **B. Bocklund***, R.A. Otis*, Z.-K. Liu (2018, May). *Software Workshop*: pycalphad and ESPEI. CALPHAD XLVII, Juriquilla, Mexico.
3. **B. Bocklund***, A. Egorov, A. Obaied, R.A. Otis, I. Roslayakova, Z.-K. Liu (2018, May). ESPEI for Efficient Database Development, Modification and Uncertainty Quantification. CALPHAD XLVII, Juriquilla, Mexico.
2. **B. Bocklund**, R.A. Otis*, Z.-K. Liu (2018, March). *Software Workshop*: pycalphad and ESPEI. TMS 2018 Annual Meeting, Phoenix, AZ.
1. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2018, March). Thermodynamic Modeling with Uncertainty Quantification and its Implications for Additive Manufacturing. TMS 2018 Annual Meeting, Phoenix, AZ.

* *presenter*