

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
 - 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

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

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

- 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
 - Helen R. and Van H. Leichter Graduate Fellowship recipient 2016
 - MSU College of Engineering Endowed Opportunity Fund scholarship recipient 2015
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Publications

10. **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, *Submitted*
9. S. Zomorodpoosh, **B. Bocklund**, A. Obaied, R. Otis, Z.-K. Liu, I. Roslyakova, Statistical approach for automated weighting of datasets: Application to heat capacity data, *Submitted*
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 Accepted* (2019).
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

7. **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.
6. Invited: **B. Bocklund***, R.A. Otis, Z.-K. Liu (2019, October). Automated CALPHAD modeling and uncertainty quantification of a ternary system using ESPEI. Materials Science and Technology 2019, Portland, OR.
5. 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.
4. **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.
3. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2018, October). Computational Tools for the Automated Development of a Cr-Fe-Ni-Ti-V CALPHAD Database. Materials Science and Technology 2018, Columbus, OH.
2. **B. Bocklund***, A. Egorov, A. Obaied, R.A. Otis, I. Roslyakova, Z.-K. Liu (2018, May). ESPEI for Efficient Database Development, Modification and Uncertainty Quantification. CALPHAD XLVII, Juriquilla, Mexico.
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.

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