

Research Experience

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

 - Developer of pycalphad and ESPEI, open research and education software for computational thermodynamics
 - Developer of atomate, a computational tool for high-throughput, first-principles DFT calculations with VASP
 - Mentor 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
 - Developed Rp Plotter, a GUI-based Python application for data analysis and visualization
 - Participated in a 10 week professional development course

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
 - Used Solidworks to create a 3D printed model for the deionization cell apparatus
 - Participated in a 10 week professional development course

East Lansing, MI
2014 – 2015

Teaching Experience

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

 - (Spring 2020) MatSE 410: Phase Relations in Materials Systems
 - o Developed problem sets for homework
 - o Graded homework and exams
 - (Spring 2018) MatSE 404/BME 444: Surfaces and the Biological Response to Materials
 - o Developed and graded problems for homework and exams
 - (Spring 2017) MatSE 462: General Properties Laboratory in Materials
 - o Independently taught and graded assignments for two lab sections of 10 students
 - o Instructed students on using techniques for characterizing mechanical, electrical and optical properties

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

 - Mentored 3 classes, interacting with over 250 students
 - Responsible for grading assignments and quizzes, promoting learning, and proctoring exams
 - o EGR 100: Introduction to Engineering Design
 - o EGR 102: Introduction to Engineering Modeling
 - o EGR 291: Spatial Visualization

East Lansing, MI
2015 – 2016

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

- pycalphad: Runner Up, NASA Software of the Year (SoY) award 2019
- Honorable Mention, National Science Foundation Graduate Research Fellowship Program 2018
- Outstanding Contribution in Reviewing - *CALPHAD* 2017
- Helen R. and Van H. Leichliter Graduate Fellowship recipient 2016
- MSU College of Engineering Endowed Opportunity Fund scholarship recipient 2015

Publications

- 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).
- **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*
- 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.
- **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.
- 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.
- 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.
- 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
- 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.
- 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

- 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.
- 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.
- **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.
- **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.
- **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.
- **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

Technical Skills

Software Developed: pycalphad (pycalphad.org), ESPEI (espei.org), atomate (atomate.org)
Computational Tools and Software: Python, MATLAB, VASP, Thermo-Calc, MongoDB