Brandon Bocklund

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Research Experience

• Phases Research Lab, Pennsylvania State University

University Park, PA

2016 - Present

- 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

NASA Jet Propulsion Lab

La Cañada Flintridge, CA

05/2017 - 08/2017

Graduate Research Intern (Mentors: Richard Otis, Peter Dillon)

NASA Space Technology Research Fellow (Advisor: Zi-Kui Liu)

- Used computational thermodynamics to develop bulk metallic glass alloy composition specifications
- Developed a model for oxygen tolerance in bulk metallic glasses
- Solid State Ionics Laboratory, Michigan State University

East Lansing, MI

2015 - 2016

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
- Composite Materials & Structures Center, Michigan State University

Undergraduate Research Assistant (Advisor: Lawrence T. Drzal)

East Lansing, MI

2014 - 2015

- 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

Teaching Experience

• Department of Materials Science and Engineering, Pennsylvania State University Teaching Assistant University Park, PA

2017

- MatSE 404/BME 444: Surfaces and the Biological Response to Materials
 - o Developed and graded problems for homework and exams
- MatSE 462: General Properties Laboratory in Materials
 - o Independently taught and graded assignments for two lab sections of 10 students
 - Instructed students on using techniques for characterizing mechanical, electrical and optical properties

• College of Engineering, Michigan State University Undergraduate Lab Mentor

East Lansing, MI

2015 - 2016

- 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

Education

• Pennsylvania State University

University Park, PA

Ph.D., Materials Science and Engineering; Graduate Minor, Computational Materials

2016 - Present

- 3.73 GPA

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

• Michigan State University

East Lansing, MI

B.S. Materials Science and Engineering

2012 - 2016

- 3.56 GPA
- Dean's List, 5 semesters

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).
- 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

Technical Skills

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