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

East Lansing, MI

Undergraduate Research Assistant (Advisor: Lawrence T. Drzal)

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 462: General Properties Laboratory in Materials
 - 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
 - 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

- 3.86 GPA
- NASA Space Technology Research Fellow (2018 Present)
- Honorable Mention, National Science Foundation Graduate Research Fellowship Program (2018)
- NSF Research Trainee in the CoMET Program (dftcomet.psu.edu) (2016 2018)
- Helen R. and Van H. Leichliter Graduate Fellowship recipient (2016)

• Michigan State University

East Lansing, MI

2012 - 2016

B.S. Materials Science and Engineering

- 3.56 GPA
- Dean's List, 5 semesters
- MSU College of Engineering Endowed Opportunity Fund scholarship recipient (2015 2016)

Publications

- Bobbio, L.D., **Bocklund**, **B.**, Otis, R, Borgonia, J.P., Dillon, R.P., Shapiro, A.A., McEnerney, B., Liu, Z.-K., Beese, A.M. 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**, **1031-1036 (2018).** doi: 10.1016/j.jallcom.2018.01.156
- Mathew, K., Montoya, J.H., Faghaninia, A., Dwarakanath, S., Aykol, M., Tang, H., Chu, I., Smidt, T., **Bocklund, B.**, Horton, M., Dagdelen, J., Wood, B., Liu, Z.-K., Neaton, J., Ong, S.P., Persson, K., Jain, A. 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
- Smith, N. D., Marker, C., **Bocklund**, **B.**, Orabona, N., Lichtenstein, T., Gesualdi, J., Nigl, T., Liu, Z.-K., Kim, H. Thermodynamic Assessment of the Strontium-Antimony Binary System via Electromotive Force Measurements Supported by First-Principles Calculations and CALPHAD Modeling. *Submitted*.
- Bobbio, L.D., Bocklund, B., Otis, R., Borgonia, J.P., Dillon, R.P., Shapiro, A.A., McEnerney, Bryan, Liu, Z.-K., Beese, A.M. Experimental analysis and thermodynamic calculations of an additively manufactured functionally graded material of V to Invar 36. Accepted.
- Marker, C., Higgins, O., Smith, N., **Bocklund**, **B.**, Kim, H., Liu, Z.-K. Thermodynamic modeling of the Ba-Sb system from first-principles calculations. *In preparation*.
- **Bocklund**, **B.**, Otis, R. A., Egorov, A., Roslyakova, I., Liu, Z.-K. ESPEI for efficient database development, modification and uncertainty quantification: application to the Cu-Mg system. *In preparation*.

Technical Skills

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