Brandon Bocklund

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Research Experience

- **Phases Research Lab, Pennsylvania State University** — University Park, PA
  NASA Space Technology Research Fellow (Advisor: Zi-Kui Liu) — 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
  Graduate Research Intern (Mentors: Richard Otis, Peter Dillon) — 05/2017 – 08/2017

  - 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
  Undergraduate Research Assistant (Advisor: Jason D. Nicholas) — 2015 – 2016

  - 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** — University Park, PA
  Teaching Assistant — 2017

  - MatSE 404/BME 444: Surfaces and the Biological Response to Materials
    - Developed and graded problems for homework and exams
  - 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** — East Lansing, MI
  Undergraduate Lab Mentor — 2015 – 2016

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