Brandon Bocklund

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Research Experience

• Phases Research Lab, Pennsylvania State University

University Park, PA

2016 - Present

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

• NASA Jet Propulsion Lab

La Cañada Flintridge, CA

05/2017 - 08/2017

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

- Fabricated and improved the performance of solid oxide fuel cells

- Designed a graphene nanoplatlet-based capacitive deionization cell

• Solid State Ionics Laboratory, Michigan State University

East Lansing, MI

2015 - 2016

- Undergraduate Research Assistant (Advisor: Jason D. Nicholas)
 - Characterized fuel cells with EIS, XRD, and SEM
- Composite Materials & Structures Center, Michigan State University

East Lansing, MI

2014 - 2015

- Undergraduate Research Assistant (Advisor: Lawrence T. Drzal)
 - Characterized graphene nanoplatelet papers using scanning electron microscopy

Teaching Experience

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

2016 - Present

- (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

• College of Engineering, Michigan State University

East Lansing, MI

Undergraduate Lab Mentor

2015 - 2016

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

Education

• Pennsylvania State University

University Park, PA

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

2016 - Present

- 3.74 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

• 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. Leichliter Graduate Fellowship recipient, Pennsylvania State University

2016

2015

• College of Engineering Endowed Opportunity Fund scholarship recipient, Michigan State University

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** 69 (2020) 101762. doi: 10.1016/j.calphad.2020.101762.
- 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 ES-PEI. TMS 2020 Annual Meeting, San Diego, CA.
- 6. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2019, October) *Invited*. Automated CALPHAD modeling and uncertanty 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 CALHPAD Database. Materials Science and Technology 2018, Columbus, OH.
- 2. **B. Bocklund***, A. Egorov, A. Obaied, R.A. Otis, I. Roslayakova, 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 Quantifiation and its Implicitaions for Additive Manufacturing. TMS 2018 Annual Meeting, Phoenix, AZ.

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