Brandon Bocklund

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Research Experience

- **Materials Science Division, Lawrence Livermore National Laboratory** **Livermore, CA**
  Postdoctoral Researcher (Supervisor: Aurélien Perron) *2021 – Present*
  - Modeling phase transformations through atomistic, mesoscale, and machine learning techniques
  - Led development of Materials Acceleration Platform (MAP) used by several LLNL projects
  - Contributed to three successful LDRD proposals (23-ERD-005, 23-ERD-034, and 24-FS-030) and two externally funded proposals (FY24-26 NA-22 and FY24 Critical Materials Institute)
  - Team member for TAOS (The Alloy Optimization Software), an LLNL commercialized product
  - Selected to Cohort 5 of the Critical Materials Institute Leadership Academy (2024)
  - MSD Seminar Organizing Team member (2022 – *Present*)
  - Supervised a Materials and Chemistry Institute (MaCI) summer graduate student intern (A.M. Krajewski, 2022 and 2023)
  - Completed ALE3D Introductory Course (2022)
- **Phases Research Lab, Pennsylvania State University** **University Park, PA**
  NASA Space Technology Research Fellow (Advisor: Zi-Kui Liu) *2016 – 2021*
  - 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
  - Co-organized and delivered two workshops on "Software Tools from Atomistics to Phase Diagrams" with over 140 total attendees (November 10-11, 2020 and December 8-9, 2020)
  - Mentored 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
- **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

Teaching Experience

- **Department of Materials Science and Engineering, Pennsylvania State University** **University Park, PA**
  Teaching Assistant *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 – 2021*
  - 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

- LLNL PLS FY24 Winter Directorate Award: Excellence in Publication *2024*
- Robert E. Newnham Award for Research Excellence, Pennsylvania State University *2020*
- Larry Kaufman Scholarship, Calphad XLIX Conference *2020*
- 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*
- Travel Award for iMATSE Graduate Students, Pennsylvania State University *2017*
- Helen R. and Van H. Leichliter Graduate Fellowship, Pennsylvania State University *2016*
- College of Engineering Endowed Opportunity Fund scholarship, Michigan State University *2015*

Publications

30. H. Sun, B. Pan, Z. Yang, A. Krajewski, **B. Bocklund**, S.-L. Shang, J. Li, A.M. Beese, Z.-K. Liu, MaterialsMap:A CALPHAD-Based Tool to Design Composition Pathways through feasibility map for Desired Dissimilar Materials, demonstrated with RSW Joining of Ag-Al-Cu, *Submitted*.

29. N. Ury, **B. Bocklund**, A. Perron, K. Bertsch, Automated Path Planning for Functionally Graded Materials Considering Phase Stability and Solidification Behavior, *Submitted*.

28. **B. Bocklund**, A. Perron, J.T. McKeown, K. Bertsch, Implementation of an Extensible Property Modeling Framework in ESPEI with Applications to Molar Volume and Elastic Stiffness Models, **Calphad** *Accepted*.

27. S. Liu, **B. Bocklund**, J. Diffenderfer, S. Chaganti, B. Kailkhura, S. McCall, B. Gallagher, A. Perron, J.T. McKeown, A Comparative Study of Predicting High Entropy Alloy Phase Fractions with Traditional Machine Learning and Deep Neural Networks, **npj Computational Materials** *Accepted*.

26. C. Kunselman, **B. Bocklund**, A. van de Walle, R. Otis, R. Arroyave, Analytically Differentiable Metrics for Phase Stability, **Calphad** *Accepted*.

25. B. Tonyali, H. Sun, **B. Bocklund**, J.P. Borgonia, R.A. Otis, S.-L. Shang, Z.-K. Liu, A.M. Beese, Additively manufactured Ni-20Cr to V functionally graded material: Computational predictions and experimental verification of phase formations, **Journal of Alloys and Compounds** 985 (2024) 174011. doi: 10.1016/j.jallcom.2024.174011.

24. J. Shittu, C.J. Rietema, M. Juhasz, B. Ellyson, K.L.M. Elder, **B. Bocklund**, Z.C. Sims, T.T. Li, H.B. Henderson, J. Berry, A. Samanta, T. Voisin, A.A. Baker, S.K. McCall, A.P. Perron, J.T. McKeown, Microstructural, phase, and thermophysical stability of CrMoNbV refractory multi-principal element alloys, **Journal of Alloys and Compounds** 997 (2024) 173349. doi: 10.1016/j.jallcom.2023.173349.

23. H. Sun, S.L-. Shang, R. Gong, **B. Bocklund**, A.M. Beese, Z.-K. Liu, Thermodynamic modeling of the Nb-Ni system with uncertainty quantification using PyCalphad and ESPEI, **Calphad** 82 (2023) 102563. doi: 10.1016/j.calphad.2023.102563.

22. J. Paz Soldan Palma, R. Gong, **B. Bocklund**, R. Otis, M. Poschmann, M. Piro, S. Shahbazi, T.G. Levitskaia, S. Hu, N.D. Smith, Y. Wang, H. Kim, Z.-K. Liu, S.-L. Shang, Thermodynamic modeling with uncertainty quantification using the modified quasichemical model in quadruplet approximation: Implementation into PyCalphad and ESPEI, **Calphad** 83 (2023) 102618. doi: 10.1016/j.calphad.2023.102618.

21. K.L.M. Elder, J. Berry, **B. Bocklund**, J. Shittu, C.J. Rietema, H.B. Henderson, S.K. McCall, A. Perron, J.T. McKeown, Computational discovery of ultra-strong, stable, and lightweight refractory multi-principal element alloys. Part II: comprehensive ternary design and validation, **npj Computational Materials** 9 (2023) 88. doi: 10.1038/s41524-023-01031-6.

20. K.L.M. Elder, J. Berry, **B. Bocklund**, S.K. McCall, A. Perron, J.T. McKeown, Computational discovery of ultra-strong, stable, and lightweight refractory multi-principal element alloys. Part I: design principles and rapid down-selection, **npj Computational Materials** 9 (2023) 84. doi: 10.1038/s41524-023-01030-7.

19. M. Ostrowska, P. Riani, **B. Bocklund**, Z.-K. Liu, G. Cacciamani, Thermodynamic modeling of the Al-Co-Cr-Fe-Ni high entropy alloys supported by key experiments, **Journal of Alloys and Compounds** 897 (2022) 162722. doi: 10.1016/j.jallcom.2021.162722

18. I. Sanghyeok, S.-L. Shang, N.D. Smith, A.M. Krajewski, T. Lichtenstein, S. Hui, **B. Bocklund**, Z.-K. Liu, H. Kim, Thermodynamic properties of the Nd-Bi system via emf measurements, DFT calculations, machine learning, and CALPHAD modeling, **Acta Materialia** 223 (2022) 117448. doi: 10.1016/j.actamat.2021.117448.

17. L.D. Bobbio, **B. Bocklund**, E. Simsek, R.T. Ott, M.J. Kramer, Z.-K. Liu, A.M. Beese, Design of an additively manufactured functionally graded material of 316 stainless steel and Ti-6Al-4V with Ni-20Cr, Cr, and V intermediate compositions, **Additive Manufacturing** 51 (2022) 102649. doi: 10.1016/j.addma.2022.102649.

16. Y. Wang, M. Liao, **B.J. Bocklund**, P. Gao, S.-L. Shang, H. King, A.M. Beese, L.-Q. Chen, Z.-K. Liu DFTTK: Density Functional Theory Tool Kit for High-throughput Calculations of Thermodynamic Properties at Finite Temperatures, **Calphad** 75 (2021) 102355 doi: 10.1016/j.calphad.2021.102355

15. C. Wang, S.-L. Shang, J. You, **B. Bocklund**, Y. Wang, H.-Y. Wang, Z.-K. Liu, Understanding the effect of oxygen on the glass-forming ability of Zr43Cu43Al7Be7 bulk metallic glass by ab initio molecular dynamics simulations, **Metallurgical and Materials Transactions A** 52 (2021) 2501–2511. doi: 10.1007/s11661-021-06242-4.

14. L.D. Bobbio, **B. Bocklund**, Z.-K. Liu, A.M. Beese, Tensile behavior of stainless steel 304L to Ni-20Cr functionally graded material: experimental characterization and computational simulations, **Materialia** (2021) 101151. doi: 10.1016/j.mtla.2021.101151

13. P. Vogt, F.V.E. Hensling, K. Azizie, C.S. Chang, D. Turner, J. Park, J.P. McCandless, H. Paik, **B. Bocklund**, G. Hoffman, O. Bierwagen, D. Jena, H.G. Xing, S. Mou, D.A. Muller, S.-L. Shang, Z.-K. Liu, D.G. Schlom, Adsorption-Controlled Growth of Ga2O3 by Suboxide Molecular-Beam Epitaxy, *Featured* **APL Materials** 9(3) 031101. doi: 10.1063/5.0035469.

12. R. Otis, **B. Bocklund**, Z.-K. Liu, Sensitivity estimation for calculated phase equilibria, **Journal of Materials Research** (2020) 1–11. doi: 10.1557/jmr.2020.269.

11. K.M. Adkison, S.-L. Shang, **B. Bocklund**, D. Klimm, D.G. Schlom, Z.-K. Liu, Suitability of binary oxides for molecular-beam epitaxy source materials: A comprehensive thermodynamic analysis, *Featured* **APL Materials** 8 (2020) 081110. doi: 10.1063/5.00131

10. S. Zomorodpoosh, **B. Bocklund**, A. Obaied, R.A. Otis, Z.-K. Liu, I. Roslyakova, Statistical approach for automated weighting of datasets: Application to heat capacity data, **CALPHAD** 71 (2020) 101994. doi: 10.1016/j.calphad.2020.101994.

9. **B. Bocklund**, L.D. Bobbio, R.A. Otis, A.M. Beese, Z.-K. Liu, Experimental validation of Scheil-Gulliver simulations for the gradient path planning in additive manufactured functionally graded materials, **Materialia** 11 (2020) 100689. doi: 10.1016/j.mtla.2020.100689.

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

20. **B. Bocklund***, A. Perron, K. Bertsch (2024, May). Implementation of an extensible property modeling framework in ESPEI. Calphad LI, Stockholm, Sweden.

19. **B. Bocklund***, N. Ury, A. Perron (2024, April). Progress in thermodynamic modeling of molten salt separation processes for NdCl3. CMI Hub Meeting, Golden, CO.

18. **B. Bocklund***, R.A. Otis* (2023, June). *Software Workshop:* PyCalphad and ESPEI. CALPHAD 50, Boston, MA.

17. **B. Bocklund***, A. Perron (2023, March). Rapidly generating Calphad databases with high-throughput first-principles calculations. TMS 2023 Annual Meeting, San Diego, CA.

16. **B. Bocklund***, R.A. Otis* (2022, September). *Software Workshop:* PyCalphad and ESPEI. Structure and Thermodynamics of Oxides/carbides/nitrides/borides at High Temperatures (STOHT), Tempe, AZ.

15. **B. Bocklund***, R.A. Otis, A. Perron, Z.-K. Liu (2022, May). A general approach for computing the residuals between CALPHAD models and phase diagram data. Calphad XLIX, Stockholm, Sweden.

14. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2022, March). Uncertainty Quantification and Propagation in CALPHAD Modeling. TMS 2022 Annual Meeting, Anaheim, CA.

13. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2020, February). Uncertainty quantification and propagation in ICME enabled by ESPEI. TMS 2020 Annual Meeting, San Diego, CA.

12. **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.

11. **B. Bocklund**, R.A. Otis*, Z.-K. Liu (2019, June). *Software Workshop:* PyCalphad and ESPEI. CALPHAD XLVIII, Singapore.

10. 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.

9. M. Feurer, **B. Bocklund***, S. Shang, A. Beese, Z.-K. Liu (2019, June). High-Throughput Modeling of Cr-Fe-Ni Sigma Phase. CALPHAD XLVIII, Singapore.

8. **B. Bocklund***, R.A. Otis, Z.-K. Liu (2019, June). Automated CALPHAD modeling and uncertanty quantification of a ternary system using ESPEI. CALPHAD XLVIII, Singapore.

7. **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.

6. **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.

5. **B. Bocklund***, R.A. Otis*, Z.-K. Liu (2018, May). *Software Workshop:* PyCalphad and ESPEI. CALPHAD XLVII, Juriquilla, Mexico.

4. **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.

3. **B. Bocklund**, R.A. Otis*, Z.-K. Liu (2018, March). *Software Workshop:* PyCalphad and ESPEI. TMS 2018 Annual Meeting, Phoenix, AZ.

2. **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.

1. **B. Bocklund***, R.A. Otis, J. Paz Soldan-Palma, Y. Wang, Z.-K. Liu (2017, May). Automating Thermodynamic Database Development with ESPEI. 4th World Congress on Integrated Computational Materials Engineering, Ypsilanti, MI.

* *presenter*