

CHRISTOPHER J. BARTEL

cbartel@berkeley.edu | [Website \(cjbartel.github.io\)](http://Website(cjbartel.github.io))
+1 985 502 1870 | 2130 Bonar St. Apt. C Berkeley, CA 94702 USA

Research Interests

I am a computational chemical and materials engineer working to accelerate the realization of solid-state inorganic materials for energy applications. I approach this problem using *ab initio* quantum chemistry calculations and machine learning. So far, my work has addressed the design of materials for batteries, optoelectronics, solar fuels, ceramics, and catalysts. I also strive for fundamental insights into materials chemistry by working to understand and predict the stability and reactivity of solid-state materials.

Experience

Postdoctoral Scholar, University of California, Berkeley May 2019 – present
Materials Science and Engineering
Advisor: Prof. Gerbrand Ceder

Graduate Research Assistant, University of Colorado Boulder August 2014 – December 2018
Chemical Engineering
Advisors: Prof. Charles Musgrave & Prof. Alan Weimer
Thesis: *Data-driven descriptors for the thermochemistry of inorganic crystalline solids*

Education

PhD University of Colorado Boulder, Chemical Engineering 2014 – 2018
MS University of Colorado Boulder, Chemical Engineering 2014 – 2016
BS Auburn University, Chemical Engineering 2010 – 2014

Publications

17 published papers | 12 since 2019 | [Google Scholar](#)

8 × 1st author | 4 × 2nd author | 3 × corresponding author

Journals include *JACS* (1st author), *Science Advances* (1st), *Nature Comms* (1st), *Nature Materials* (2nd)

(* denotes corresponding author, + denotes equal contribution)

17. **C. Bartel***, A. Trewartha, Q. Wang, A. Dunn, A. Jain, G. Ceder*, A critical examination of compound stability predictions from machine-learned formation energies, *npj Computational Materials*, **2020**, 6, 97
16. N. Singstock, **C. Bartel**, A. Holder*, C. Musgrave*, High-throughput analysis of materials for chemical looping processes, *Advanced Energy Materials*, **2020**, 14, 2000685
15. A. Miura*, H. Ito, **C. Bartel**, W. Sun*, N. Rosero Navarro, K. Tadanaga, H. Nakata, K. Maeda, G. Ceder, Selective metathesis synthesis of MgCr₂S₄ by control of thermodynamic driving forces, *Materials Horizons*, **2020**, 7, 1310-1316
14. **C. Bartel***, J. Clary, C. Sutton, D. Vigil-Fowler, B. Goldsmith, A. Holder, C. Musgrave*, Inorganic halide double perovskites with optoelectronic properties modulated by sublattice mixing, *JACS*, **2020**, 142, 11, 5135-5145
13. J. Koettgen, **C. Bartel**, G. Ceder*, Computational investigation of chalcogenide spinel conductors for all-solid-state Mg batteries, *ChemComm*, **2020**, 56, 1952-1955
12. E. Rognerud⁺, C. Rom⁺, P. Todd, N. Singstock, **C. Bartel**, A. Holder, J. Neilson*, Kinetically controlled low-temperature solid-state metathesis of manganese nitride Mn₃N₂, *Chemistry of Materials*, **2019**, 31, 18, 7248-7254
11. W. Sun*, **C. Bartel**, E. Arca, S. Bauers, B. Matthews, B. Orvañanos, J. Tate, W. Tumas, A. Zakutayev, S. Lany, A. Holder*, G. Ceder, A map of the inorganic ternary metal nitrides, *Nature Materials*, **2019**, 18, 732-739
10. **C. Bartel**, J. Rumpitz, A. Weimer, A. Holder*, C. Musgrave*, High-throughput equilibrium analysis of active materials for solar thermochemical ammonia synthesis, *ACS Applied Materials & Interfaces*, **2019**, 11, 28, 24850-24858

9. A. Palumbo, **C. Bartel**, J. Sorli, A. Weimer*, Characterization of products derived from the high temperature flash pyrolysis of microalgae and rice hulls, *Chemical Engineering Science*, **2019**, 196, 527-537
8. **C. Bartel***, C. Sutton, B. Goldsmith, R. Ouyang, C. Musgrave, L. Ghiringhelli*, M. Scheffler, New tolerance factor to predict the stability of perovskite oxides and halides, *Science Advances*, **2019**, 5, eaav0693
7. **C. Bartel**, A. Weimer, S. Lany, C. Musgrave*, A. Holder*, The role of decomposition reactions in assessing first-principles predictions of solid stability, *npj Computational Materials*, **2019**, 5 (1), 4
6. R. O'Toole⁺, **C. Bartel**⁺, M. Kodas, A. Horrell, S. Ricote, N. Sullivan, C. Gump, C. Musgrave, A. Weimer*, Particle atomic layer deposition of alumina for sintering yttria-stabilized cubic zirconia, *Journal of the American Ceramic Society*, **2019**, 102 (5) 2283-2293
5. **C. Bartel**, S. Millican, A. Deml, J. Rumptz, W. Tumas, A. Weimer, S. Lany, V. Stevanović, C. Musgrave*, A. Holder*, Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry, *Nature Communications*, **2018**, 9, 4168
4. B. Goldsmith*, J. Esterhuizen, J. Liu, **C. Bartel**, C. Sutton, Machine learning for heterogeneous catalyst design and discovery, *AIChE Journal*, **2018**, 64 (7), 2311-2323
3. E. Arca*, S. Lany, J. Perkins, **C. Bartel**, J. Mangum, W. Sun, A. Holder, G. Ceder, B. Gorman, G. Teeter, W. Tumas, A. Zakutayev*, Redox-mediated stabilization of zinc molybdenum nitride, *JACS*, **2018**, 140 (12), 4293-4301
2. S. Zhang, E. Yu., S. Gates, W. Cassata, J. Makel, A. Thron, **C. Bartel**, A. Weimer, R. Faller, P. Stroeve, J. Tringe*, Helium interactions with alumina formed by atomic layer deposition show potential for mitigating problems with excess helium in spent nuclear fuel, *Journal of Nuclear Materials*, **2018**, 499, 301-311
1. **C. Bartel**, C. Muhich, A. Weimer*, C. Musgrave*, Aluminum nitride hydrolysis enabled by hydroxyl-mediated surface proton hopping, *ACS Applied Materials & Interfaces*, **2016**, 8 (28), 18550-18559

Teaching

Guest Lecturer (e.g., see [Lectures 17-19 on YouTube](#))

University of California, Berkeley | Materials Science and Engineering

G Thermodynamics and Phase Transformations in Solids

Fall 2019, Fall 2020

Instructor: Prof. Gerbrand Ceder (gceder@berkeley.edu)

UG Materials in Energy Technologies

Fall 2019

Instructor: Prof. Kristin Persson (kapersson@lbl.gov)

Graduate Teaching Assistant

University of Colorado Boulder | Chemical Engineering

G Analytical Methods for Chemical Engineers

Fall 2016

Instructor: Prof. Will Medlin (will.medlin@colorado.edu)

UG Chemical Engineering Thermodynamics

Fall 2014

Instructor: Prof. John Falconer (john.falconer@colorado.edu)

Proposals

Primary contributor (~50–90%) on **three funded proposals** totaling **\$1,037,658** (NSF ×3)

Significant contributor (~30%) on **one funded proposal** totaling **\$1,111,270** (DOE ×1)

4. **C. Bartel**, A. Holder (co-PI), C. Musgrave (PI), Automated Search for Materials for Ammonia Synthesis and Water Splitting, NSF Division of Chemical, Biological, Environment, and Transport Systems, Award No. 1806079, September 2018 – August 2021, **\$136,329**
3. **C. Bartel**, A. Holder (co-PI), C. Musgrave (PI), Machine Learned Free Energies of Compounds, NSF Division of Chemistry, Award No. 1800592, September 2018 – August 2021, **\$517,497**

2. S. Millican, **C. Bartel**, R. Trottier, Z. Bare, A. Holder, A. Weimer (co-PI), C. Musgrave (PI), Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced Solar Thermochemical Hydrogen Production, DOE EERE Fuel Cell Technologies Office, Award No. DE-EE000808, September 2017 – September 2020, **\$1,111,270**
1. **C. Bartel**, J. Walsh (co-PI), R. Hall (co-PI), C. Musgrave (co-PI), A. Weimer (PI), Core/Shell Sinterable Advanced Ceramic Materials Using Particle Atomic Layer Deposition, NSF Division of Civil, Mechanical and Manufacturing Innovation, Materials Engineering and Processing Program, Award No. 1563537, July 2016 – June 2019, **\$383,832**

Awards

Max S. Peters Outstanding Graduate Student Award	2019
Awarded annually to the top PhD graduate in Chemical Engineering at CU-Boulder	
DOE EFRC Team Science Competition Winner	2019
One of 6 winners from 40 EFRC teams	
University of Washington Distinguished Young Scholars Seminar	2019
One of 8 selected speakers from >100 applicants	
Department of Education GAANN Fellowship (×2)	2017, 2018
Provided full tuition and graduate stipend for 15 months	
National Science Foundation Graduate Research Fellowship	2014 – 2017
Provided full tuition and graduate stipend for 36 months	
Department of Chemical and Biological Engineering Service Award (×2)	2016, 2017
Awarded for leading the organization of volunteering and outreach events	

Outreach

Peer Reviewer	2018 – present
<i>JACS</i> , <i>Nature Communications</i> , <i>Materials Horizons</i> , <i>JMCA</i> , <i>npj Comp. Mater.</i> , and others	
Mentor for Undergraduate Research	2016 – 2019
Mentored 5 students for ~18 months each (4× Senior Thesis 7× research awards)	
Co-chair Graduate Leadership Council Service Department	2015 – 2018
Planned and led volunteering and outreach events for Chem. E. graduate department	
Tutor & Session Chair: NOMAD Summer School	2018
Hands-on course for novel materials discovery	
Student Co-organizer: Intl. Conference for Ternary and Multinary Compounds	2018
College of Engineering and Applied Sciences Graduate Mentorship Program	2017
Developed and participated in workshops to foster positive mentor-mentee relationships	

Presentations

5 invited talks ([YouTube link to #1](#))

5. **TMS 2021 Annual Meeting** | Orlando, FL | March 2021 (invitation accepted)
Talk: Towards predictive solid-state synthesis: understanding phase evolution during the formation of YBCO
4. **ASM International IMAT 2020** | Cleveland, OH | September 2020 (canceled due to COVID-19)
Talk: Is machine learning the formation energy sufficient to accelerate materials discovery?
3. **Georgia Tech Chemical & Biomolecular Engineering** | Atlanta, GA | January 13, 2020
Talk: Data-driven descriptors for solid-state materials discovery
2. **Digital Solar Redox Materials Design Workshop** | Berkeley, CA | August 12, 2019
Talk: Machine learning for the prediction of material properties
1. **University of Washington Chemical Engineering (DYSS)** | Seattle, WA | July 1, 2019
Talk: Predictive descriptors for the stability of solid-state materials

Presented 25 contributed talks (includes AIChE, MRS, ACS, APS, EMRS, and others)

References

Advisors

1. **Prof. Gerbrand Ceder**

Daniel M. Tellep Distinguished Professor in Engineering
University of California, Berkeley | Materials Science and Engineering
Senior Faculty Scientist
Lawrence Berkeley National Laboratory | Materials Sciences Division
gceder@berkeley.edu | +1 510 486 7193

2. **Prof. Charles Musgrave**

Robert H. Davis Professor and Associate Dean of Graduate Education
University of Colorado Boulder | Chemical and Biological Engineering
charles.musgrave@colorado.edu | +1 303 735 0411

3. **Prof. Alan Weimer**

Melvin E. and Virginia M. Clark Professor
University of Colorado Boulder | Chemical and Biological Engineering
alan.weimer@colorado.edu | +1 303 492 3759

Collaborators

1. **Prof. Bryan Goldsmith**

Dow Corning Assistant Professor
Chemical Engineering | University of Michigan
bgoldsm@umich.edu | +1 734 764 3627

2. **Dr. Aaron Holder**

Solid State Theory and Computational Chemistry Scientist
National Renewable Energy Laboratory | Materials and Chemical Science and Technology
Assistant Professor
University of Colorado Boulder | Chemical and Biological Engineering
aaron.holder@colorado.edu | +1 303 735 0754