Christopher J. Bartel

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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 — 2019 – present
Materials Science and Engineering
Advisor: Prof. Gerbrand Ceder

Graduate Research Assistant, University of Colorado Boulder — 2014 – 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
BS Auburn University, Chemical Engineering — 2010 – 2014

Publications

25 peer-reviewed papers | 20 since Jan. 2019 | Google Scholar
10× 1st author | 6× 2nd author | 4× corresponding author
e.g., *Sci. Adv.* (1st author), *Nat. Commun.* (1st), *JACS* (1st), *Adv. Mater.* (co-1st), *Nat. Mater.* (2nd)

(* denotes corresponding author, $^{+}$ denotes equal contribution)

25. B. Ouyang^{+}, J. Wang^{+}, T. He, **C. Bartel**, H. Huo, Y. Wang, V. Lacivita, H. Kim, G. Ceder*, Synthetic accessibility and stability rules of NASICONs, *Nature Communications*, **2021**, Accepted

24. J. Hancock, K. Griffith, Y. Choi, **C. Bartel**, S. Lapidus, J. Vaughey, G. Ceder, K. Poeppelmeier*, Expanding the ambient-pressure phase space of $CaFe_2O_4$-type sodium post spinel host-guest compounds, *ACS Organic and Inorganic Au*, **2021**, ASAP Article (*invited*)

23. L. Blanc^{+}, **C. Bartel**$^{+}$, Ha. Kim, Y. Tian, Hy. Kim, A. Miura, G. Ceder*, L. Nazar*, Toward the development of a high-voltage Mg cathode using a chromium sulfide host, *ACS Materials Letters*, **2021**, 3, 1213-1220

22. L. Yin, B. Kwon, Y. Choi, **C. Bartel**, M. Yang, C. Liao, B. Key, G. Ceder, S. Lapidus*, Operando X-ray diffraction studies of the Mg-ion migration mechanisms in spinel cathodes for rechargeable Mg-ion batteries, *Journal of the American Chemical Society*, **2021**, 143, 28, 10649-10658

21. N. Szymanski, Y. Zeng, H. Huo, **C. Bartel***, H. Kim*, G. Ceder*, Toward autonomous design and synthesis of novel inorganic materials, *Materials Horizons*, **2021**, 8, 2169-2198 (*invited*)

20. N. Szymanski, **C. Bartel**, Y. Zeng, Q. Tu, G. Ceder*, Probabilistic deep learning approach to automate the interpretation of multi-phase diffraction spectra, *Chemistry of Materials*, **2021**, 33, 11, 4204-4215

19. A. Miura^{+}*, **C. Bartel**$^{+}$, Y. Goto, Y. Mizuguchi, C. Moriyoshi, Y. Kuroiwa, Y. Wang, T. Yaguchi, M. Shirai, M. Nagao, N. Rosero-Navarro, K. Tadanaga, G. Ceder, W. Sun*, Observing and modeling the sequential pairwise reactions that drive solid-state ceramic synthesis, *Advanced Materials*, **2021**, 33, 24, 2100312

18. J. Koettgen, **C. Bartel**, J. Shen, K. Persson, G. Ceder*, First-principles study of $CaB_{12}H_{12}$ as a potential solid-state conductor for Ca, *Physical Chemistry Chemical Physics*, **2020**, 22 (47), 27600-27604

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 $MgCr_2S_4$ 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, *Journal of the American Chemical Society*, **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 Mn_3N_2, *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. Rumptz, 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 (*invited*)

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 (*invited* | *cover*)

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, *Journal of the American Chemical Society*, **2018**, 140 (12), 4293-4301 (*cover*)

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, 2020, 2021
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, *D3SC: 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**

Primary contributor on **6 High Performance Computing** proposals to DOE-BES (NERSC), DOE-EERE (Eagle), and NSF (XSEDE) totaling >**30M CPU/GPU hours**

Awards

Outstanding Reviewer for *Materials Horizons* 2020
One of 10 selected for number, timeliness, and quality of reviews (link)

Max S. Peters Outstanding Graduate Student Award 2019
Awarded annually to the top Ph.D. graduate in Chemical Engineering at CU-Boulder

DOE EFRC Team Science Competition Winner 2019
One of 6 winners from 40 EFRC teams (link)

University of Washington Distinguished Young Scholars Seminar 2019
One of 8 selected speakers from >100 applicants (link)

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
Journals: *Energy Environ Sci*, *JACS*, *Nat Commun*, *Mater Horiz*, *ACS Energy Lett*, *Chem Mater*, *JMCA*, *npj Comp Mater*, *J Phys Chem*, *Patterns*, *PCCP*, *Appl Phys Lett*, *Catal Sci Tech*, and others
Agencies: US DOE Basic Energy Sciences (CMS, CCS)

Mentor for Graduate Research 2019 – present
Supervising 3 Ph.D. students (4 co-authored papers published so far)

Mentor for Undergraduate Research 2016 – 2019
Supervised 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

7 invited talks (YouTube links to talks at UW in 2019 and TMS in 2021)

7. **TMS 2022 Annual Meeting** | Anaheim, CA | March 2022
   The challenge of machine learning the stability of materials
6. **TMS 2021 Annual Meeting** | Orlando, FL (virtual) | March 18, 2021
   Towards predictive synthesis: understanding phase evolution during the formation of YBCO (link)
5. **Northeastern University Chemical Engineering** | Boston, MA (virtual) | February 22, 2021
   Data-driven descriptors for solid-state materials discovery
4. **ASM International IMAT 2020** | Cleveland, OH | September 2020 (canceled due to COVID-19)
   Is machine learning the formation energy sufficient to accelerate materials discovery?
3. **Georgia Tech Chemical & Biomolecular Engineering** | Atlanta, GA | January 13, 2020
   Data-driven descriptors for solid-state materials discovery
2. **Digital Solar Redox Materials Design Workshop** | Berkeley, CA | August 12, 2019
   Machine learning for the prediction of material properties
1. **University of Washington Chemical Engineering (DYSS)** | Seattle, WA | July 1, 2019
   Predictive descriptors for the stability of solid-state materials (link)

Presented 27 contributed talks (includes AIChE, MRS, ACS, APS, and others)

References

1. **Prof. Gerbrand Ceder**
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   University of California, Berkeley | Materials Science and Engineering
   Senior Faculty Scientist
   Lawrence Berkeley National Laboratory | Materials Sciences Division
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2. **Prof. Charles Musgrave**
   Robert H. Davis Professor and *Associate Dean of Graduate Education*
   University of Colorado Boulder | Chemical and Biological Engineering
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3. **Prof. Alan Weimer**
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