

CHRISTOPHER J. BARTEL

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Appointments

Assistant Professor , University of Minnesota Chemical Engineering and Materials Science (link) Chemical Physics, <i>Graduate Faculty</i> (link) Data Science Initiative, <i>Affiliate</i> (link)	2022 – present
Postdoctoral Scholar , University of California, Berkeley Materials Science and Engineering (link) Advisor: Prof. Gerbrand Ceder	2019 – 2022
Graduate Research Assistant , University of Colorado Boulder Chemical Engineering (link) Advisors: Prof. Charles Musgrave & Prof. Alan Weimer Thesis: <i>Data-driven descriptors for the thermochemistry of inorganic crystalline solids</i>	2014 – 2018

Education

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

Honors & Awards

Scialog Fellow in Negative Emission Science Selected as one of ~50 early-career faculty fellows (link)	2023
Outstanding Reviewer for <i>Materials Horizons</i> One of 10 selected for number, timeliness, and quality of reviews (link)	2020
Max S. Peters Outstanding Graduate Student Award Awarded annually to the top Ph.D. graduate in Chemical Engineering at CU-Boulder	2019
DOE EFRC Team Science Competition Winner One of 6 winners from 40 EFRC teams (link)	2019
University of Washington Distinguished Young Scholars Seminar One of 8 selected speakers from >100 applicants (link)	2019
Department of Education GAANN Fellowship (×2) Provided full tuition and graduate stipend for 15 months	2017, 2018
National Science Foundation Graduate Research Fellowship Provided full tuition and graduate stipend for 36 months	2014 – 2017
Department of Chemical and Biological Engineering Service Award (×2) Awarded for leading the organization of volunteering and outreach events	2016, 2017
Auburn University Presidential Scholarship Provided full tuition support for 4 years	2010 – 2014

Publications

[Google Scholar](#) | [ORCID:0000-0002-5198-5036](#)

* denotes corresponding author, + denotes equal contribution

40. N. Szymanski, Z. Lun, J. Liu, Z. Cai, E. Self, **C. Bartel**, J. Nanda, B. Ouyang, G. Ceder*, Modeling short-range order in disordered rocksalt cathodes by pair distribution function analysis, *Chemistry of Materials*, **2023**, 35, 13, 49224934
39. T. He, H. Ho, **C. Bartel**, Z. Wang, K. Cruse, G. Ceder*, Precursor recommendation for inorganic synthesis by machine learning materials similarity from scientific literature, *Science Advances*, **2023**, 9, 23, adg8180

38. M. Kothakonda, A. Kaplan, E. Isaacs, **C. Bartel**, J. Furness, J. Ning, C. Wolverton, J. Perdew, J. Sun*, Testing the r²SCAN density functional for the thermodynamic stability of solids with and without a van der Waals correction, *ACS Materials Au*, **2023**, 3, 2, 102-111
37. N. Szymanski, **C. Bartel**, Y. Zeng, M. Diallo, H. Kim, G. Ceder*, Adaptive X-ray diffraction with automatic phase identification, *npj Computational Materials*, **2023**, 9 (1), 31
36. M. Cosby, **C. Bartel**, A. Corrao, A. Yakovenko, L. Gallington, G. Ceder, P. Khalifah*, Thermodynamic and kinetic barriers limiting solid state reactions resolved through in situ synchrotron studies of lithium halide salts, *Chemistry of Materials*, **2023**, 35, 3, 917-926
35. L. Blanc⁺, Y. Choi⁺, A. Shyamsunder, B. Key, S. Lapidus, C. Li, L. Yin, B. Gwalani, Y. Xiao, **C. Bartel**, G. Ceder*, L. Nazar*, Phase stability and kinetics of topotactic dual Ca²⁺-Na⁺ ion electrochemistry in NaSICON NaV₂(PO₄)₃, *Chemistry of Materials*, **2023**, 35, 2, 468-481
34. R. Sherbondy⁺, R. Smaha⁺, **C. Bartel**, M. Holtz, K. Talley, B. Levy-Wendt, C. Perkins, S. Eley, A. Zakutayev, G. Brennecke*, High-throughput selection and experimental realization of two new Ce-based nitride perovskites: CeMoN₃ and CeWN₃, *Chemistry of Materials*, **2022**, 34, 15, 6883-6893
33. H. Huo, **C. Bartel**, T. He, A. Trewartha, A. Dunn, B. Ouyang, A. Jain, G. Ceder*, Machine-learning rationalization and prediction of solid-state synthesis conditions, *Chemistry of Materials*, **2022**, 34, 16, 7323-7336
32. N. Szymanski⁺, Y. Zeng⁺, T. Bennett, S. Patil, J. Keum, E. Self, J. Bai, Z. Cai, R. Giovone, B. Ouyang, F. Wang, **C. Bartel**, R. Clement, W. Tong, J. Nanda, G. Ceder*, Understanding the fluorination of disordered rocksalt cathodes through rational exploration of synthesis pathways, *Chemistry of Materials*, **2022**, 34, 15, 7015-7028
31. **C. Bartel***, Review of computational approaches to predict the thermodynamic stability of inorganic solids, *Journal of Materials Science*, **2022**, 57:10475-10498 (invited)
30. R. O'Toole, C. Hill, P. Buur, **C. Bartel**, C. Gump, C. Musgrave, A. Weimer*, Hydrolysis protection and sintering of aluminum nitride powders with yttria nanofilms, *Journal of the American Ceramic Society*, **2022**, 105, 5, 3123-3127
29. B.J. Kwon*, L. Yin, **C. Bartel**, K. Kumar, P. Parajuli, J. Gim, S. Kim, R. Klie, S. Lapidus, B. Key, G. Ceder, J. Cabana*, Intercalation of Ca into a highly defective oxide at room temperature, *Chemistry of Materials*, **2022**, 34, 2, 836-846
28. R. Kingsbury, A. Gupta, **C. Bartel**, J. Munro, S. Dwaraknath, M. Horton, K. Persson*, Performance comparison of r²SCAN and SCAN metaGGA density functionals for solid materials via an automated, high-throughput computational workflow, *Physical Review Materials*, **2022**, 6, 013801
27. Y. Chen, **C. Bartel**, M. Avdeev, Y. Zhang, P. Zhong, G. Zeng, Z. Cai, H. Kim, H. Ji*, G. Ceder*, Solid-state Ca ion diffusion in Ca_{1.5}Ba_{0.5}Si₅O₃N₆, *Chemistry of Materials*, **2022**, 34, 1, 128-139
26. J. Hancock, K. Griffith, Y. Choi, **C. Bartel**, S. Lapidus, J. Vaughey, G. Ceder, K. Poeppelmeier*, Expanding the ambient-pressure phase space of CaFe₂O₄-type sodium post spinel host-guest compounds, *ACS Organic and Inorganic Au*, **2022**, 2, 1, 8-22 (invited | cover)
25. H. Park*, **C. Bartel**, G. Ceder, P. Zapol*, Layered transition metal oxides as Ca intercalation cathodes: a systematic first-principles evaluation, *Advanced Energy Materials*, **2021**, 11, 48, 2101698
24. 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**, 12, 5752
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 CaB₁₂H₁₂ 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 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, *Journal of the American Chemical Society*, **2020**, *142*, 11, 5135-5145 (*correction*)
13. J. Koettgen, **C. Bartel**, G. Ceder*, Computational investigation of chalcogenide spinel conductors for all-solid-state Mg batteries, *Chemical Communications*, **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. 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

2 other publications

2. **C. Bartel**, R. O'Toole, M. Kodas, A. Weimer, Core-shell ceramic particle colloidal gel and solid oxide fuel cell electrolyte, **2023**, US Patent No. 11,613,502 B2
1. **C. Bartel***, Data-centric approach to improve machine learning models for inorganic materials, *Patterns*, **2021**, 2, 11, 100361 (invited preview)

Teaching

Course Instructor

University of Minnesota — Chemical Engineering and Materials Science

ChEn 3005 – Transport Phenomena: Momentum and Heat

Fall 2022 (5.5), *Fall 2023*

ChEn/MatS 5802 – Applied Machine Learning in Chemical and Materials Engineering

Spring 2023 (5.8), *Spring 2024*

Ratings in parentheses are average Student Rating of Teaching scores for “Instructor Overall” (max = 6.0)

Service (external)

Peer Reviewer

2018 – present

Journals:

Energy and Environmental Science, Advanced Materials, Journal of the American Chemical Society, Nature Communications, Materials Horizons, Matter, ACS Energy Letters, Chemistry of Materials, ACS Materials Letters, Chemical Science, npj Computational Materials, Digital Discovery, PRX Energy, Patterns, Journal of Chemical Theory and Computation, Journal of Materials Chemistry A, Accounts of Materials Research, Journal of Physical Chemistry C, Physical Chemistry Chemical Physics, Applied Physics Letters, APL Materials, Catalysis Science and Technology, Journal of Materials Science, Computational Materials Science, Journal of Applied Physics, Materials Today Energy, and others

Agencies:

US Department of Energy Office of Science (BES-CMS, BES-CCS, BES-MSE, ASCR, SCGSR)
ACS Petroleum Research Fund (DNI, UNI)

Early Career Advisory Board Member

2023 – 2025

Materials Today Energy

Co-organizer | Peter O. Stahl Advanced Design Forum ([link](#))

2023, 2024

Session co-organizer & co-chair | AIChE Annual Meeting

CoMSEF: Machine Learning for Hard and Soft Materials

2023

MESD: Accelerated Discovery of Inorganic Materials

2023

Co-organizer | UMN Data Science Initiative ML for Materials Workshop

2023

Instructor & Co-organizer | i-CoMSE Summer School

2023

Machine Learning for Molecular Sciences ([link](#))

Co-organizer | Industrial Perspectives on Data Science in Chem. and Adv. Mater. ([link](#)) 2022

Service (UMN)

Research Supervision	2022 – present
Bartel Research Group	
<i>Postdoctoral Researchers</i>	
Dr. Madhulika Mazumder (<i>CEMS</i> , 2023–)	
<i>Graduate researchers (PhD)</i>	
Yi-Ting (Chris) Cheng (<i>ChEn</i> , 2022–)	
Kyle Noordhoek (<i>MatS</i> , 2022–)	
Jane Schlesinger (<i>ChemPhys</i> , 2022–)	
<i>Undergraduate researchers</i>	
Sean Sullivan (<i>ChEn</i> , 2022–)	
Simon Hjaltason (<i>ChEn</i> , 2023–)	
Graduate Admissions Committee	2022 – present
Ph.D. Materials Science (link)	
M.S. Data Science for Chemical Engineering and Materials Science (link)	
PhD Thesis Defense Committees	2022 – present
PhD Qualifying Exam Committees	2022 – present
Faculty Mentor for Graduate students	2022 – present
Faculty Advisor for Undergraduate students	2023 – present
Faculty Search Committee (CEMS)	2023 – 2024
Faculty judge UMN Chemistry Graduate Student Research Symposium	2023

Invited Presentations

28. **MRS Spring Meeting** | Seattle, WA | April 22, 2024
Integrating Machine Learning and Simulations for Materials Modeling
27. **ACS Midwest-Great Lakes Regional Meeting** | St. Louis, MO | October 18, 2023
Theoretical Chemistry
26. **Society of Engineering Science Annual Meeting** | Minneapolis, MN | October 8, 2023
Interatomic Models in Materials Simulations: Theory, Standards, Infrastructure, and Applications
25. **Mach Conference** | Baltimore, MD | April 7, 2023
Systems for Fitting, Uncertainty Quantification, Selection, and Use of Interatomic Models
24. **UMN Electrical and Computer Engineering** | Minneapolis, MN | March 17, 2023
Magnetic Seminar
23. **IIT Delhi: Tryst** | Delhi, India (virtual) | February 15, 2023
Department of Chemical Engineering Learning Webinar
22. **AIChE Annual Meeting** | Phoenix, AZ | November 18, 2022
Fundamental Theory and Characterizations for Optoelectronic Materials
21. **UMN Aerospace Engineering & Mechanics** | Minneapolis, MN | October 4, 2022
Solid Mechanics Research Seminar
20. **UMN CSE Data Science Initiative** | Minneapolis, MN | September 28, 2022
Machine Learning Seminar Series
19. **U of Toronto Chemical Engineering & Applied Chemistry** | Toronto, ON | March 22, 2022
Department seminar
18. **UC Irvine Materials Science and Engineering** | Irvine, CA | March 17, 2022
Department seminar
17. **University of Utah Chemical Engineering** | Salt Lake City, UT | March 10, 2022
Department seminar

16. **U of Maryland Chemical & Biomolecular Engineering** | College Park, MD | March 7, 2022
Department seminar
15. **TMS Annual Meeting** | Anaheim, CA | February 28, 2022
Phase Stability, Transformations, and Reactive Formation in Electronic Materials XXI
14. **U Minnesota Chemical Engineering & Materials Science** | Minneapolis, MN | Feb 22, 2022
Department seminar
13. **OSU Chemical & Biological Engineering** | Columbus, OH (*virtual*) | February 15, 2022
Department seminar
12. **NC State University Chemical & Biomolecular Engineering** | Raleigh, NC | February 9, 2022
Department seminar
11. **University of Utah Chemistry** | Salt Lake City, UT (*virtual*) | January 31, 2022
Department seminar
10. **University of Florida Chemical Engineering** | Gainesville, FL | January 24, 2022
Department seminar
9. **University of Virginia Chemical Engineering** | Charlottesville, VA | January 20, 2022
Department seminar
8. **Indiana University Chemistry** | Bloomington, IN | January 12, 2022
Department seminar
7. **SUNY Buffalo Materials Design and Innovation** | Buffalo, NY | December 17, 2021
Department seminar
6. **TMS Annual Meeting** | Orlando, FL (*virtual*) | March 18, 2021
Phase Stability, Transformations, and Reactive Formation in Electronic Materials X ([link](#))
5. **Northeastern University Chemical Engineering** | Boston, MA (*virtual*) | February 19, 2021
Department seminar
4. **ASM International IMAT** | Cleveland, OH | September 2020 (canceled due to COVID-19)
Materials 4.0: Materials Information in the Product Life Cycle
3. **Georgia Tech Chemical & Biomolecular Engineering** | Atlanta, GA | January 13, 2020
Department seminar
2. **Lawrence Berkeley National Laboratory** | Berkeley, CA | August 12, 2019
Digital Solar Redox Materials Design Workshop
1. **University of Washington Chemical Engineering** | Seattle, WA | July 1, 2019
Distinguished Young Scholars Seminar Series ([link](#))