Nathan J. Szymanski

Assistant Professor · Materials Science and Engineering

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Research Interests

I am a materials scientist working to advance the development of sustainable energy technologies by integrating computational and experimental methods. My work combines *ab-initio* quantum chemistry, machine learning, and Monte Carlo simulations to model inorganic materials synthesis. By pairing these techniques with *in-situ* characterization and AI-driven data analysis, my group streamlines the process between initial discovery and commercialization of next-generation materials for batteries and fuel cells.

Education

University of California, Berkeley — *Berkeley, CA*
PhD Materials Science and Engineering — *2019 - 2024*
- Advisor: Prof. Gerbrand Ceder

University of Toledo — *Toledo, OH*
BS Physics and Applied Mathematics — *2015 - 2019*

Professional Experience

2025-	**Assistant Professor**, Materials Science and Engineering, University of California, Los Angeles
2024-2025	**Postdoctoral Researcher**, Chemical Engineering and Materials Science, University of Minnesota
2019-2024	**Graduate Research Assistant**, Materials Science and Engineering, University of California, Berkeley
2023-2024	**Graduate Teaching Assistant**, Graduate-level Thermodynamics, University of California, Berkeley

Publications

1. **N. J. Szymanski**, A. Smith, P. Daoutidis, and C. J. Bartel, Topological descriptors for the electron density of inorganic solids. ACS Materials Letters 7, 2158–2164 (2025).

2. H. Kim, K. Jun, **N. J. Szymanski**, V. Sai, Z. Cai, M. Crafton, G.-H. Lee, S. E. Trask, F. Babbe, Y.-W. Byeon, P. Zhong, D. Lee, B. Park, W. Jung, B. D. McCloskey, and W. Yang, Screening and Development of Sacrificial Cathode Additives for Lithium-Ion Batteries, Advanced Energy Materials, 2403946 (2025).

3. **N. J. Szymanski** and C. J. Bartel, Establishing baselines for the generative discovery of inorganic crystals, preprint available on arXiv (2025).

4. V. S. Avvaru, T. Li, G.-H. Lee, Y.-W. Byeon, K. P. Koirala, O. J. Marques, S. Jeong, **N. J. Szymanski**, M. Kunz, F. Babbe, V. Battaglia, B. D. McCloskey, J. N. Weker, C. Wang, W. Yang, R. J. Clément, and H. Kim, Alternative Solid State Synthesis Route for Highly Fluorinated Disordered Rocksalt Cathode Materials for High Energy Lithium Ion Batteries, Advanced Energy Materials, 2500492 (2025).

5. Y. Chen, X. Zhao, K. Chen, K. P. Koirala, R. Giovine, X. Yang, S. Wang, **N. J. Szymanski**, S. Xiong, Z. Lun, H. Ji, C. Wang, J. Bai, F. Wang, B. Ouyang, G. Ceder, Coherent-Precipitation-Stabilized Phase Formation in Over-Stoichiometric Rocksalt-Type Li Superionic Conductors, Advanced Materials, 2416342 (2024).

6. **N. J. Szymanski** Y.-W. Byeon, Y. Sun, Y. Zeng, J. Bai, M. Kunz, C. J. Bartel, H. Kim, and & G. Ceder, Quantifying the regime of thermodynamic control in solid-state reactions. *Science Advances* 10, eadp3309 (2024).

7. **N. J. Szymanski** & C. J. Bartel, Computationally Guided Synthesis of Battery Materials. *ACS Energy Letters* 9, 2902 (2024).

8. Y. Fei, B. Rendy, R. Kumar, O. Dartsi, H. P. Sahasrabuddhe, M. J. McDermott, Z. Wang, **N. J. Szymanski**, L. N. Walters, D. Milsted, Y. Zeng, A. Jain, G. Ceder, AlabOS: a Python-based reconfigurable workflow management framework for autonomous laboratories. *Digital Discovery*, Advance Article (2024).

9. S. Wang, **N. J. Szymanski**, Y. Fei, Y. Zeng, M. Whittacker, & G. Ceder, Direct Lithium Extraction from α-Spodumene through Solid-State Reactions for Sustainable Li_2CO_3 Production. *Inorganic Chemistry* (2024).

10. **N. J. Szymanski**, S. Fu, E. Persson, & G. Ceder, Integrated analysis of X-ray diffraction patterns and pair distribution functions for machine-learned phase identification. *npj Computational Materials* 10, 45 (2024).

11. Y. Zeng* and **N. J. Szymanski***, T. He, K. Jun, L. C. Gallington, H. Huo, C. J. Bartel, B. Ouyang, & G. Ceder, Selective formation of metastable polymorphs in solid-state synthesis. *Science Advances* 10, eadj5431 (2024).

12. L. Rettenberger, **N. J. Szymanski**, Y. Zeng, J. Scheutzke, S. Wang, G. Ceder, & M. Reischl, Uncertainty-aware particle segmentation for electron microscopy at varied length scales. *npj Computational Materials* 10, 124 (2024).

13. **N. J. Szymanski***, B. Rendy*, Y. Fei*, R. E. Kumar*, T. He, D. Milsted, M. J. McDermott, M. Gallant, E. D. Cubuk, A. Merchant, H. Kim, A. Jain, C. J. Bartel, K. Persson, Y. Zeng, & G. Ceder, An autonomous laboratory for the accelerated synthesis of novel materials. *Nature* 624, 86-91 (2023).

14. **N. J. Szymanski***, P. Nevatia*, C. J. Bartel, Y. Zeng, & G. Ceder, Autonomous and dynamic precursor selection for solid-state materials synthesis. *Nature Communications* 14, 6956 (2023).

15. **N. J. Szymanski**, C. J. Bartel, Y. Zeng, M. Diallo, H. Kim, & G. Ceder, Adaptively driven X-ray diffraction guided by machine learning for autonomous phase identification. *npj Computational Materials* 9, 31 (2023).

16. **N. J. Szymanski**, S. Fu, E. Persson, & G. Ceder, Z. Lun, J. Liu, E. C. Self, C. J. Bartel, J. Nanda, B. Ouyang, & G. Ceder, Modeling Short-Range Order in Disordered Rocksalt Cathodes by Pair Distribution Function Analysis. *Chemistry of Materials* 35, 4922-4934 (2023).

17. Y. W. Byeon, M. J. Gong, Z. Cai, Y. Sun, **N. J. Szymanski**, J. Bai, D. H. Seo, & H. Kim, Effects of cation and anion substitution in $KVPO_4F$ for K-ion batteries. *Energy Storage Materials* 57, 81-91 (2023).

18. **N. J. Szymanski**, Y. Zeng, T. Bennett, S. Patil, J. K. Keum, E. C. Self, J. Bai, Z. Cai, R. Giovine, B. Ouyang, F. Wang, C. J. Bartel, R. J. Clément, W. Tong, J. Nanda, & G. Ceder, Understanding the Fluorination of Disordered Rocksalt Cathodes through Rational Exploration of Synthesis Pathways. *Chemistry of Materials* 34, 7015-7028 (2022).

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

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

21. I. Khare, **N. J. Szymanski**, D. Gall, & R. Irving, Electronic, optical, and thermoelectric properties of sodium pnictogen chalcogenides: A first principles study. *Computational Materials Science* 183, 109818 (2020).

22. **N. J. Szymanski***, L. N. Walters*, D. Puggionio, & J. Rondinelli, Design of heteroanionic MoON exhibiting a Peierls metal-insulator transition. *Physical Review Letters* 123, 236402 (2019).

23. **N. J. Szymanski**, V. Adhikari, M. A. Willard, P. Sarin, D. Gall, & S. V. Khare, Prediction of improved magnetization and stability in $Fe_{16}N_2$ through alloying. *Journal of Applied Physics* 127, 093903 (2019).

24. **N. J. Szymanski**, I. Khatri, J. G. Amar, D. Gall, & S. V. Khare, Unconventional superconductivity in 3d rocksalt transition metal carbides. *Journal of Materials Chemistry C* 7, 12619 (2019).

25. **N. J. Szymanski**, V. Adhikari, I. Khatri, D. Gall, & S. V. Khare, Improved optoelectronic properties in $CdSe_xTe_{1-x}$ through controlled composition and short-range order. *Solar Energy* 194, 742 (2019).

26. V. Adhikari, **N. J. Szymanski**, I. Khatri, D. Gall, & S. V. Khare, First principles investigation into the phase stability and enhanced hardness of TiN-ScN and TiN-YN alloys. *Thin Solid Films* 688, 137284 (2019).

27. **N. J. Szymanski**, L. N. Walters, O. Hellman, D. Gall, & S. V. Khare, Dynamical stabilization in delafossite nitrides for solar energy conversion. *Journal of Materials Chemistry A* 6, 20852 (2018).

28. **N. J. Szymanski**, Z. T. Y. Liu, T. Alderson, N. J. Podraza, P. Sarin, & S. V. Khare, Electronic and optical properties of vanadium oxides from first principles. *Computational Materials Science* 146, 310 (2018).

29. V. Adhikari, Z. T. Y. Liu, **N. J. Szymanski**, I. Khatri, D. Gall, P. Sarin, & S. V. Khare, First-principles study of mechanical and magnetic properties of transition metal (M) nitrides in the cubic M_4N structure. *Journal of Physics and Chemistry of Solids* 120C, 197 (2018).

Patents Pending

2024 **Li extraction from spodumene**, A method of synthesizing Li precursors directly from hard minerals.

Awards & Fellowships

2024	**Didier de Fontaine Award in Theory and Computation** , UC Berkeley	*$ 2,000*
2023	**Jane Lewis Fellowship for Research in Mining**, UC Berkeley	*$ 40,000*
	Vedensky Award in Process Metallurgy, UC Berkeley	*$ 1,000*
2019	**NSF Graduate Research Fellowship**, National Science Foundation	*$ 108,000*
2018	**Barry Goldwater Fellowship**, United States Congress	*$ 7,500*

Software

CrysTopo. Tools for the topological analysis of DFT-computed charge densities.

MatGen-Baselines. A package to benchmark generative AI for materials discovery.

XRD-AutoAnalyzer. A package to automate phase identification from multi-phase XRD patterns.

ARROWS. A decision-making algorithm designed to optimize solid-state synthesis procedures.

AdaptiveXRD. Software that integrates automated XRD analysis with in-line steering of measurements.

Invited Talks

Summer 2025. *How computed thermodynamics can inform materials synthesis*. MTSM, Madison, WI.

Summer 2024. *Creating a self-driving lab for the development of new materials*. 3M Research Seminar, Minneapolis, MN.

Spring 2024. *Automating materials synthesis with robotics, DFT, and ML*. MACH Conference, Annapolis, MD.

Fall 2023. *An autonomous laboratory for inorganic materials synthesis*. Future Labs Workshop, UC Santa Barbara.

Spring 2023. *Using ML to adaptively steer XRD measurements*. Workshop on ML for X-ray and neutron scattering, LBNL.

Contributed Talks

Sprint 2025. *Understanding the growth of rutile Ge oxides in hybrid MBE*. Spring APS Global Physics Summit, Anaheim, CA.

Summer 2024. *Quantifying the regime of thermodynamic control in solid reactions*. Solid-State GRS, New London, NH.

Summer 2024. *Using robotics and ML to synthesize novel materials*. Stahl Research Forum, Minneapolis, MN

Summer 2023. *Characterizing short-range order in Li-ion cathode materials*. ICMAT Conference, Singapore.

Spring 2023. *How neural networks can be used to drive XRD measurements*. Spring MRS, San Fransisco, CA.

Spring 2022. *Data-driven decision making to optimize materials synthesis*. Spring MRS, Honolulu, HI.

Spring 2022. *An overview of automation in the characterization of inorganic materials*. JCESR Research Seminar, LBNL.

Fall 2021. *Probabilistic machine learning as a tool for the analysis of diffraction patterns*. Fall MRS, Boston, MA.

Teaching Experience

2024-2025 **Machine learning for Chemical Engineering and Materials Science**, Guest Lecturer (slides)
2023 **Thermodynamics and Phase Transformations**, Graduate Teaching Assistant
2019 **Introduction to Mathematical Proofs**, Undergraduate Teaching Assistant

Outreach & Professional Development

Service and Outreach

2024 **ASM Materials Camp**, University of Minnesota, Volunteer for 3D printing demonstration
2024 **High School STEM Outreach**, Spring Lake Park Schools, Presenter and coordinator
2018 **Feed My Starving Children**, University of Toledo, Event planner for a fundraising event

Development

2023 Teaching Conference, UC Berkeley, Interactive workshop on fostering inclusion and diversity in graduate courses.

2019 Conference for Women in Physics, Michigan State University, Discussion on how to improve gender equity in Physics.

Peer Review

Reviewed papers in several journals including *Journal of the American Chemical Society*, *npj Computational Materials*, *Chemistry of Materials*, *ACS Applied Electronic Materials*, *Physical Chemistry Chemical Physics*, and *Materials Today Energy*