Steven B. **Torrisi**

Research Scientist · Physicist & Materials Scientist

Toyota Research Institute, 4400 El Camino Real, Los Altos CA

https://stevetorr.github.io/ | stevetorr | stevenbtorrisi | Google Scholar | Last updated: August 30, 2025

Education

Harvard University *Cambridge, MA*

Ph.D. in Physics (Secondary Field in Computational Science & Engineering) *2021*

- Advisors: Boris Kozinsky, Efthimios Kaxiras. Dissertation Title: Materials Informatics for Catalyst Stability & Functionality
- Collaborators: Kristin Persson (UCB Materials Science & Engineering), Eun-ah Kim (Cornell Physics), Jason Brickner (Northwestern Biology).
- Served as a major developer of open-source packages like FLARE and InterMatch.

University of Rochester *Rochester, NY*

B.S. in Physics (with Highest Distinction); B.A. in Math (With Distinction) *2016*

Professional Experience

Toyota Research Institute

Senior Research Scientist *2021 - Present*

- Published as a **corresponding author in the NeurIPS AI for Accelerated Materials Design workshop and npj Computational Materials,** and **as a co-author in over a dozen total publications** since joining TRI in 2021.
- Authored multiple patents.
- Was the primary liaison for six university research programs at universities including MIT, Stanford, UC Berkeley, Columbia, and Northwestern.
- Jointly designed and lead the Synthesis Advanced Research Challenge, a consortium of university projects focused on the challenge of predictive solid-state synthesis.

Selected Honors & Awards

2023	**Royal Society of Chemistry 2022 Outstanding Reviewer** Digital Discovery	*RSC*
2017	**DOE Computational Science Graduate Fellowship**	*Department of Energy*
2017	**National Defense Science and Engineering Graduate Fellowship (Declined)**	*Department of Defense*
2017	**Wallace Noyes Fellowship** Harvard Physics Department	*Harvard University*
2016	**Elected to Phi Beta Kappa, Iota Chapter**	*University of Rochester*
2015	**Barry M. Goldwater Scholarship**	*US Government*
2012	**Renaissance & Global Scholarship** Full-tuition scholarship awarded on admission	*University of Rochester*
2012	**Alan & Jane Handler Scholarship** Full room and board/book scholarship awarded on admission	*University of Rochester*

Publications

(As of August 30, 2025): **Citations: 1425, h-index: 15, Lead/Co-Lead/Last/Corresponding Author: 8**

29. J. Huang, Z. Wang J. Liang XY Li, J. Pietryga, Z Ye, P. T. Smith, A. Kulaksizoglu, C.R. McCormick, J. Kim, B. Peng, Z. Liu, K. Xie, **Steven B. Torrisi**, J.H. Montoya, G. Wu, E.H. Sargent, C A. Mirkin "Accelerating the Pace of Oxygen Evolution Reaction Catalyst Discovery through Megalibraries", **Journal of the American Chemical Society**, 2025, DOI

28. T. Liu, **Steven B. Torrisi**, C. Wolverton "Short-Range Order and Li_x $\mathrm{TM4}-x$ Probability Maps for Disordered Rocksalt Cathodes" arXiv

27. T. Liu, A. Salgado-Casanova, S. Yubuchi, B. Baldassarri, M. Aykol, J. Yoshida, H. Yamasaki, Y. Zhu, ***Steven B. Torrisi,** C. Wolverton "Tailored Ordering enables high-capacity cathode materials", arXiv. *Corresponding author.

26. B. van Vlijmen, V.N. Lam, P.A. Asinger, X. Cui, J. Schaeffer, A. Geslin, D. Ganapathi, S. Sun, P.K. Herring, C.B. Gopal, N. Geise, H.D. Deng, H.L. Thaman, S.D. Kang, **Steven B. Torrisi**, A. Trewartha, A. Anapolsky, B.D. Storey, W.E. Gent, R.D. Braatz, W.C. Chueh "Aging matrix visualizes complexity of battery aging across hundreds of cycling protocols" **Energy & Environmental Science**, 2025, 18, 6641-6654 DOI.

25. T. Na Narong, Z.N. Zachko, ***Steven B. Torrisi,*** S.J.L. Billinge, "Interpretable multimodal machine learning analysis of X-ray absorption near-edge spectra and pair distribution functions", **npj Computational Materials**, 2025, 11, 1, 98, DOI. *Corresponding author.

24. T. Liu, D. Gaines II, H. Kim, A. Salgado-Casanova, **Steven B Torrisi**, Chris Wolverton "Anomalous Reversal of Stability in Mo-containing Oxides: A Difficult Case Exhibiting Sensitivity to DFT+ U and Distortion" **Physical Review Materials**, 2025, 9, 055402 DOI

23. K. Sheriff, R. Freitas, A. Trewartha, **S. Torrisi**, "Simultaneous Discovery of Reaction Coordinates and Committor Functions Using Equivariant Graph Neural Networks", AI for Accelerated Materials Design-NeurIPS 2024, Link

22. X. Cui, S.D. Kang, S. Wang, J.A. Rose, H. Lian, A. Geslin, **S.B. Torrisi**, M.Z. Bazant, S. Sun, W.C. Chueh, "Data-driven analysis of battery formation reveals the role of electrode utilization in extending cycle life", **Joule**, 2024, 8, 11, 3072-3087 DOI

21. J.H. Montoya, C. Grimley, M. Aykol, C. Ophus, H. Sternlicht, B.H. Savitzky, A.M. Minor, **Steven B Torrisi**, J. Goedjen, C.C. Chung, A.H. Comstock, S. Sun, "How the AI-assisted discovery and synthesis of a ternary oxide highlights capability gaps in materials science", **Chemical Science**, 2024, 15, 5660-5673. DOI

20. E. Gerber, **S.B. Torrisi**, S. Shabani, E. Seewald, J. Pack, J.E. Hoffman, C.R. Dean, A.N. Pasupathy, E.A. Kim, "High-Throughput Ab Initio Design of Atomic Interfaces using InterMatch," **Nature Communications**, 2023. 14, 7921

19. B. Baldassarri, J. He, and A. Gopakumar, and S. Griesemer, A.J.A. Salgado-Casanova, Adolfo T.C. Liu, **S.B. Torrisi** , C. Wolverton, "Oxygen Vacancy Formation Energy in Metal Oxides: High-Throughput Computational Studies and Machine-Learning Predictions", **Chemistry of Materials**, Vol. 35, 24, pp. 10619-10634, 2023

18. C.J. Owen, **S.B. Torrisi***, Y. Xie, S. Batzner, J. Coulter, A. Musaelian, L. Sun, B. Kozinsky, "Complexity of Many-Body Interactions in Transition Metals via Machine-Learned Force Fields from the TM23 Data Set," **NPJ Computational Materials**, 2024, 10, 1, 92. DOI. *Co-first author.

17. M. Ansari, **S.B. Torrisi**, A. Trewartha, S. Sun, "History-Agnostic Battery Degradation Inference," **Journal of Energy Storage**, 2024, 81, 110279. DOI

16. A. Khajeh, D. Schweigert, **S.B. Torrisi**, L. Hung, B.D. Storey, H.K. Kwon, "Early prediction of ion transport properties in solid polymer electrolytes using machine learning and system behavior-based descriptors of molecular dynamics simulations," **Macromolecules**, vol. 56, no. 13, p. 4787-4799, 2023.

15. **S.B. Torrisi**, M.Z. Bazant, A.E. Cohen, M.G. Cho, J.S. Hummelshøj, L. Hung, G. Kamat, A. Khajeh, A. Kolluru, X. Lei, *et al.*, "Materials cartography: A forward-looking perspective on materials representation and devising better maps," **APL Machine Learning**, vol. 1, no. 2, 2023.

14. J.H. Montoya, M. Aykol, A. Anapolsky, C.B. Gopal, P.K. Herring, J.S. Hummelshøj, L. Hung, H.K. Kwon, D. Schweigert, S. Sun, S.K. Suram, **S.B. Torrisi**, A. Trewartha, B.D. Storey, "Toward autonomous materials research: Recent progress and future challenges," **Applied Physics Reviews**, vol. 9, no. 1, 2022.

13. M.B. Stevens, M. Anand, M.E. Kreider, E.K. Price, J.Z. Zeledón, L. Wang, J. Peng, H. Li, J.M. Gregoire, J.S. Hummelshøj, T.F. Jaramillo, H. Jia, J.K. Nørskov, Y. Roman-Leshkov, Y. Shao-Horn, B.D. Storey, **S.B. Torrisi**, J.H. Montoya, "New challenges in oxygen reduction catalysis: a consortium retrospective to inform future research," **Energy & Environmental Science**, vol. 15, no. 9, p. 3775-3794, 2022.

12. N. Marcella, J.S. Lim, A.M. Płonka, G. Yan, C.J. Owen, J.E.S. van der Hoeven, A.C. Foucher, H.T. Ngan, **S.B. Torrisi**, N.S. Marinkovic, E.A. Stach, J.F. Weaver, J. Aizenberg, P. Sautet, B. Kozinsky, A.I. Frenkel, "Decoding reactive structures in dilute alloy catalysts," **Nature Communications**, vol. 13, no. 1, p. 832, 2022.

11. A. Palizhati, **S.B. Torrisi**, M. Aykol, S.K. Suram, J.S. Hummelshøj, J.H. Montoya, "Agents for sequential learning using multiple-fidelity data," **Scientific Reports**, vol. 12, no. 1, p. 4694, 2022.

10. M.C. Sumner, **S.B. Torrisi**, D.G. Brickner, J.H. Brickner, "Random sub-diffusion and capture of genes by the nuclear pore reduces dynamics and coordinates inter-chromosomal movement," **eLife**, vol. 10, p. e66238, 2021.

9. D.T. Larson, W. Chen, **S.B. Torrisi**, J. Coulter, S. Fang, E. Kaxiras, "Effects of structural distortions on the electronic structure of T-type transition metal dichalcogenides," **Physical Review B**, vol. 102, no. 4, p. 045128,

2020.

8. T.D. Rhone, W. Chen, S. Desai, **S.B. Torrisi**, D.T. Larson, A. Yacoby, E. Kaxiras, "Data-driven studies of magnetic two-dimensional materials," **Scientific Reports**, vol. 10, no. 1, p. 15795, 2020.
7. J. Vandermause, **S.B. Torrisi**, S. Batzner, Y. Xie, L. Sun, A.M. Kolpak, B. Kozinsky, "On-the-fly active learning of interpretable Bayesian force fields for atomistic rare events," **npj Computational Materials**, vol. 6, no. 1, p. 20, 2020.
6. **S.B. Torrisi**, A.K. Singh, J.H. Montoya, T. Biswas, K.A. Persson, "Two-dimensional forms of robust CO2 reduction photocatalysts," **npj 2D Materials and Applications**, vol. 4, no. 1, p. 24, 2020.
5. **S.B. Torrisi**, M.R. Carbone, B.A. Rohr, J.H. Montoya, Y. Ha, J. Yano, S.K. Suram, L. Hung, "Random forest machine learning models for interpretable X-ray absorption near-edge structure spectrum-property relationships," **npj Computational Materials**, vol. 6, no. 1, p. 109, 2020.
4. G.A. Tritsaris, S. Carr, Z. Zhu, Y. Xie, **S.B. Torrisi**, J. Tang, M. Mattheakis, D.T. Larson, E. Kaxiras, "Electronic structure calculations of twisted multi-layer graphene superlattices," **2D Materials**, vol. 7, no. 3, p. 035028, 2020.
3. S. Carr, D. Massatt, **S.B. Torrisi**, P. Cazeaux, M. Luskin, E. Kaxiras, "Relaxation and domain formation in incommensurate two-dimensional heterostructures," **Physical Review B**, vol. 98, no. 22, p. 224102, 2018.
2. F. Warmer, **S.B. Torrisi**, C.D. Beidler, A. Dinklage, Y. Feng, J. Geiger, F. Schauer, Y. Turkin, R. Wolf, P. Xanthopoulos, *et al.*, "System code analysis of HELIAS-type fusion reactor and economic comparison with tokamaks," **IEEE Transactions on Plasma Science**, vol. 44, no. 9, p. 1576-1585, 2016.
1. **S.B. Torrisi**, J.W. Britton, J.G. Bohnet, J.J. Bollinger, "Perpendicular laser cooling with a rotating-wall potential in a Penning trap," **Physical Review A**, vol. 93, no. 4, p. 043421, 2016.

Patents & Patent Applications

6. **S.B.J. Torrisi**, J.H. Montoya - "Piezoelectric material delivery devices and material delivery systems with piezoelectric material delivery devices", US Patent App 18/582,768, 2025
5. **S.B.J. Torrisi**, C. Wolverton, Y. Zhu, T.-C. Liu, B. Baldassarri, A. Salgado-Casanova, M. Aykol, S. Yubuchi, H. Yamasaki, J. Yoshida, "Disordered rock-salt battery cathode composition and syntheses thereof", US Patent App. 18/897,372, 2025
4. **S.B.J. Torrisi**, C. Wolverton, Y. Zhu, T.-C. Liu, B. Baldassarri, A. Salgado-Casanova, M. Aykol, S. Yubuchi, H. Yamasaki, J. Yoshida, "Lithium-chromium-iron disordered rock-salt battery cathode materials and syntheses thereof", US Patent App. 18/897,588, 2025
3. M. Ansari, S. Sun, **S.B.J. Torrisi**, A.E. Trewartha, "History-agnostic battery degradation inference", US Patent App. 18/121,171, 2024
2. **S. Torrisi**, J.H. Montoya, "Chemical compound recommendation process," US Patent App. 17/739,932, 2023.
1. J.S. Hummelshøj, S.K. Suram,**S. Torrisi**, "State Learning in an Event-Sourced Architecture for Materials Provenance (ESAMP)", US Patent App. 17/830,202, 2023

Textbook Chapters & Technical Reports

2. **S.B. Torrisi**, J.M. Gregoire, J. Yano, M.R. Carbone, C.P. Gomes, L. Hung, S.K. Suram, "Artificial intelligence for materials spectroscopy," in *Accelerated Materials Discovery: How to Use Artificial Intelligence to Speed Up Development*, p. 65, Walter de Gruyter GmbH & Co KG, 2022.
1. **S. Torrisi**, F. Warmer, "Design of an N-dimensional parameter scanner for the systems code PROCESS," Max-Planck-Institut für Plasmaphysik, 2014.

Peer Review

Nature Communications (1) **NPJ Computational Materials**(2) **Digital Discovery** (2)

Applied Physics Letters- Machine Learning (2) **Scientific Data** (1) **ICLR ML4Materials** (1) **The Journal of Chemical Physics** (1)

Invited Talks

2025	**Advanced Light Source User Workshop**	*Berkeley, CA*
2025	**NIST Artificial Intelligence for Materials Science Workshop**	*Rockland, MD*
2025	**UC Merced Mechanical Engineering Seminar**	*Merced, CA*
2024	**Materials Research Society, Spring 2024** Materials Cartography: The Role of Materials Representation	*Seattle, WA*
2024	**Materials Research Society, Spring 2024** Battery Informatics in Devices & Discovery	*Seattle, WA*
2024	**Telluride Science Research Conference: Machine Learning and Informatics for Chemistry and Materials**	*Telluride, CO*
2024	**Fordham University Chemistry Seminar**	*New York, NY*
2024	**Brookhaven National Laboratory Seminar**	*Upton, NY*
2024	**Columbia University Special Seminar**	*New York, NY*
2023	**Telluride Science Research Conference: Machine Learning and Informatics for Chemistry and Materials**	*Telluride, CO*
2023	**SUNCAT Summer School at Stanford University** Computational Representations of Materials	*Palo Alto, CA*
2023	**Argonne National Labs ML for Science Seminar** Computational Representations of Materials	*Virtual*
2022	**Guest Lecture, Numerical Methods and ML For ChE at Carnegie Mellon University** ML in Materials Discovery Design and Characterization	*Pittsburgh, PA*
2023	**Scott Institute for Energy Innovation, Carnegie Mellon University** ML in Materials Discovery Design and Characterization	*Pittsburgh, PA*
2021	**LBNL Advanced Light Source User Meeting** Machine Learning on XAS Data Analysis	*Virtual*
2021	**MIT CRIBB Seminar** Which parts matter? Interpretable random forest models for X-Ray absorption spectra	*Virtual*
2021	**Brown Theoretical Physics Center IDEA Talk** Which parts matter? Interpretable random forest models for X-Ray absorption spectra	*Virtual*

Other Honors & Awards

2021	**Harvard Physics White Prize for Excellence in Teaching**	*Harvard University*
2020	**Winner of Communicate Your Science & Engineering Contest** "Shazam for Atoms"	*Krell Institute*
2019	**Harvard University Star Family Prize for Excellence in Sophomore Advising**	*Harvard University*
2016	**Purcell Fellowship** Harvard Physics Department	*Harvard University*
2016	**NSF Graduate Research Fellowship Honorable Mention**	*Nat'l Science Foundation*
2016	**Janet Fogg Prize** For dedicated service to the Department of Physics and Astronomy	*University of Rochester*
2016	**Physics Department Teaching Award**	*University of Rochester*
2015	**Reporter Award** Funded attendance at the OSA Frontiers in Optics conference	*Society of Physics Students*
2015	**Winner Outstanding Presentation, SURF Colloquium**	*NIST*
2015	**Winner of U. Rochester Undergraduate Writing Competition** Natural & Applied Sciences Category	*University of Rochester*
2014	**Physics Department Honors Physics Prize**	*University of Rochester*
2014	**RISE Scholarship** Funded research in Germany at the Max Planck Institute for Plasma Physics	*DAAD*
2014	**Leadership Award** University of Rochester Debate Union	*University of Rochester*
2013	**Iota Book Award** Phi Beta Kappa Chapter	*University of Rochester*
2012	**Research and Innovation Grant**	*University of Rochester*

Submitted Conference Presentations

Advanced Automotive Battery Congress — *2023*

Battery Informatics from Low Context to Full History: Supervised, Unsupervised, and Interpretable ML — *San Diego, CA*

MRS Fall Meeting — *2021*

Benchmarking Descriptors Models and Systems for Many-Body Machine Learned Force Fields in Molten Transition Metals — *Boston, MA*

ACS Spring Meeting *2021*
Random forest models for X-Ray absorption spectra *Virtual*

MRS Spring Meeting *2021*
Random forest models for X-Ray absorption spectra *Virtual*

APS March Meeting *2021*
Insights on Bimetallic Surface Dynamics via Automatically Trained Gaussian Process ML Potentials *Virtual*

APS March Meeting *2019*
Two Dimensional Phases of Robust CO_2 Reduction Photocatalysts *Boston, MA*

MRS Spring *2019*
Two Dimensional Phases of Robust CO_2 Reduction Photocatalysts *Phoenix, CA*

APS March Meeting *2018*
Behavior of Weyl Semimetals in the Hydrodynamic Electron Transport Regime *Los Angeles, CA*

Frontiers in Optics undergraduate symposium *2015*
Updated Modeling of Doppler Laser Cooling in a Penning Trap *San Jose, CA*

Rochester Symposium for Physics Students at SUNY Oswego *2015*
Light Pulse Control of Quantum Information in Bose-Einstein Condensates *Oswego, NY*

Syracuse Undergraduate Research Day *2014*
A Light Pulse Control System for Quantum Information in Bose-Einstein Condensates *Syracuse, NY*

DAAD-RISE Scholars Conference *2014*
Mapping the Future of Fusion *Heidelberg, Germany*

Teaching Assistant Experience

Spring 2020	**PHYS12A: Mechanics & Statistical Physics**	*Harvard University*
Spring 2016	**PHY 237: Quantum Mechanics of Physical Systems**	*University of Rochester*
Fall 2015	**PHY 235W: Classical Mechanics**	*University of Rochester*
Spring 2015	**PHY 114: General Physics II: E&M and Modern Physics**	*University of Rochester*
Fall 2014	**PHY 122P: Electricity and Magnetism**	*University of Rochester*
Spring 2014	**PHY 114: General Physics II: E&M and Modern Physics**	*University of Rochester*
Fall 2013	**PHY 113: General Physics I: Intro to Mechanics**	*University of Rochester*

Skills and Interests

Computational & Technical Skills

Programming	Python (primary), C/C++, Unix Shell, MATLAB, Mathematica, Apache Spark
Software & Tools	Jupyter, NumPy, SciPy, Matplotlib, MapReduce, AWS, Slurm, LaTeX, PyCharm, Spyder
Techniques	Numerical analysis, Data visualization, Monte Carlo methods, Gaussian Processes, Machine Learning
Workflow & Environments	Process automation, HPC workflow tools (pymatgen, FireWorks, Atomate)

Productivity & Platforms

OS	Linux (Fedora), macOS, Windows
Office	Microsoft Office, OpenOffice
Typesetting	LaTeX

Affiliations and Extracurricular

Memberships	APS, MRS, Sigma Pi Sigma (ΣΠΣ)
Leadership	Peer Advisor — Physics Dept., University of Rochester (2015–2016); Events Coordinator — SPS (2013–2014)
Interests	Debate Union, Wind Symphony (Tenor Saxophone), Community Engagement (Rochester Center for Community Leadership)

Professional Engagement & Service

Advisory and Committee Service

UC Merced, Dept. of Mechanical Engineering *Merced, CA*

External Advisory Board Member *2024–Present*

Advising departmental programs and development

Northwestern University *Virtual / In-person*

Dissertation Committee Member *2023–Present*

Students: Bianca Baldassarri (Ph.D. 2023), Tzu-Chen Liu (Exp. Ph.D. 2025)

Northwestern University *Virtual / In-person*

Qualifying Exam Committee Member *2023–Present*

Students: Adolfo Salgado-Casanova (2024), Tzu-Chen Liu (2023)

Conference and Symposium Leadership

ACS Spring 2025, San Diego

Session Organizer

- *Data-driven Autonomous and Digital Discovery of Energy Technologies*

Various Conferences

Session Chair

- ACS Spring 2025, San Diego — *Data-driven Autonomous and Digital Discovery of Energy Technologies*
- MRS Spring 2024, Seattle — *Session MT03: Machine Learning for Sustainable Electronics*
- MRS Spring 2021, Virtual — *Session CT05.03: Applications I*

Educational and Outreach Activities

Women+ Of Color Project Graduate School Workshop *Cambridge, MA / Virtual*

Organizing Committee Member & Presenter *2019–2024*

Co-authored a grant, helped organize workshops advancing underrepresented women in STEM, and prepared + gave various profesional development talks

Cabot House, Harvard College *Cambridge, MA*

Resident Tutor *2017–2021*

Formally advised dozens of undergraduates on academics, careers, and life at Harvard

Cabot House, Harvard College *Cambridge, MA*

Faculty Dean Search Advisory Committee Member *2020*

Represented student voice in dean selection process

Cabot House, Harvard College *Cambridge, MA*

Host, Personal Finance Seminar *2019–2021*

Led annual seminars on personal finance for undergraduates

Science in the News — Artificial Intelligence in Materials Science *Harvard Medical School & Beacon Hill Seminars*

Public Lecture Presenter *2019*

APS Conference for Undergraduate Women in Physics *Harvard University*

Event Organizer & Volunteer *2017*

Adopt-a-Physicist Program

Mentor *2016*

University of Rochester

Physics Department Peer Adviser *2015–2016*

Guided undergraduates on course and research planning

High Schools in New York

Outreach Speaker *2015–2016*

Delivered talks on nuclear fusion and atomic physics

Physics, Optics & Astronomy Library, University of Rochester

Student Advisory Board Member *2016*

Represented undergraduates' needs to the library administration

University of Rochester

Orientation Presenter *2015*

Spoke to parents and incoming students about undergraduate research opportunities

“Research: Get Involved, Get Ahead” *University of Rochester*

Symposium Organizer *2014*

Organized event to raise visibility for undergraduates interested in participating in research