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: May 26, 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 May 26, 2025): **Citations: 1316, h-index: 14, Lead/Co-Lead/Last/Corresponding Author: 7**

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

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

3. M. Ansari, S. Sun, **S.B.J. Torrisi**, A.E. Trewartha, "History-agnostic battery degradation inference", US Patent App. 18/121,171
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	**Telluride Science Research Conference: Machine Learning and Informatics for Chemistry and Materials**	*Telluride, CO*
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