Tess Eleonora Smidt

Curriculum Vitae

tsmidt@mit.edu | blondegeek.github.io | atomicarchitects.com | 760.207.5707
77 Massachusetts Avenue, 36-647K, Cambridge, MA 02139

Research Interests

Developing neural networks from first-principles for rich data types (e.g. scientific data and geometry), chemical and material science and design, group theory and symmetry, density functional theory, scientific computing, computational geometry, computer-aided design, rapid prototyping

Education

Ph.D, Physics, University of California, Berkeley [Dissertation] 2018
M.A., Physics, University of California, Berkeley 2014
S.B., Physics with Minor in Architecture, Massachusetts Institute of Technology 2012

Research Experience and Employment

Associate Professor, Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology Fall 2025 - present

Assistant Professor, Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology Fall 2021 - Summer 2025

Luis W. Alvarez Postdoctoral Fellow, Lawrence Berkeley National Laboratory 2018 - 2021
Designing symmetry-preserving neural networks for applications across the physical sciences. Developer of `e3nn`: an open-source modular PyTorch framework for Euclidean neural networks.

PhD Software Engineering Intern, Google Accelerated Science 2017 - 2018
Designed and implemented neural networks that are equivariant to 3D rotations and translations (i.e. tensor field networks and Euclidean neural networks).

Graduate Research Assistant, Neaton Group, UC Berkeley 2012 - 2018
Performed an automated computational search for ferroelectrics using symmetry analysis, density functional theory, and scientific workflows. Helped discover and characterize two new classes of crystals, harmonic honeycomb iridates and metal-organic chalcogenide assemblies (MOChAs).

Graduate Research Assistant, Analytis Group, UC Berkeley 2012-2013
Operated some of the world's strongest magnets and most intense x-ray sources to characterize a new quantum magnetic material. Created a lab database to connect material synthesis methods with experimental data.

Undergraduate Research Assistant, Compact Muon Solenoid (CMS), MIT & CERN 2012
Conducted preliminary feasibility study of whether a new particle interaction could be detected at the Large Hadron Collider: Higgs bosons interacting with each other. Simulated particle events and detector response.

Undergraduate Research Assistant, Conrad Group, MIT & Fermilab 2009-2012
Simulated particle physics, nuclear physics, and heat transfer to design a new neutrino source. Wrote custom finite element analysis software to ensure beam target could absorb megawatts of power from bombarding protons. Designed spatially constrained 40'x6'x2' light detection system support structure for the 70-ton MicroBooNE neutrino detector.

Awards

DOE Early Career Award	2025
Schmidt Sciences AI2050 Fellow	2025
Air Force Office of Scientific Research Young Investigator (48 out of 159 faculty applicants awarded)	2024
MIT EECS Outstanding Educator (2 awarded per year out of 169 faculty)	2023
Rising Stars in Computational and Data Science, Oden Institute at UT Austin	2019
People's Choice Winner, Lawrence Berkeley National Laboratory Research SLAM (video)	2019
Luis W. Alvarez Postdoctoral Fellowship, Lawrence Berkeley National Laboratory	2018
National Science Foundation Graduate Research Fellowship	2012

Invited Conference and Workshop Talks

2025

1. Machine Learning for Physical Sciences Workshop at NeurIPS, San Diego, CA, Dec. 6th, 2025
2. BU Materials Day, Boston University, October 24th, 2025.
3. 2nd Northeast Quantum Forum (NEQT) Conference, University of New Hampshire, October 14th to 17th, 2025.
4. 6th Artificial Intelligence for Materials Science (AIMS) hosted by NIST, National Cybersecurity Center of Excellence (NCCoE), Rockville, MD, July 9-10, 2025.
5. CECAM: Machine Learning Advances for Molecular and Materials Property Prediction, University of Notre Dame July 7-9, 2025.
6. NYC Summit for AI4 Chemistry, June 25 - 27, 2025.
7. Equivariant Vision: From Theory to Practice at CVPR 2025, Jun 11-13, 2025 Nashville, TN

2024

8. The Role of Theories, Simulation, and Machine Learning in Materials Discovery, Gordon Research Conference, Newry, Maine, July 21-26, 2024.
9. Symposium on "Machine learning, simulations and experiments for ultra low-power materials and devices", Spetses, Greece, July 7-12, 2024.
10. AI≡Science: Strengthening the Bond Between the Sciences and Artificial Intelligence, Simons Institute at UC Berkeley, June 10-14, 2024.
11. Workshop on Machine Learning in Electronic-Structure Theory, IMSI at UChicago, March 25-29, 2024.
12. APS March Meeting, Session on Statistical Physics Meets ML, Minneapolis, MN, March 7, 2024

2023

13. Materials Research Society Fall Meeting, November 28, 2023.
14. MolML, MIT, November 8, 2023.
15. [Remote] Panel Discussion on Formal Methods in the Service of Science, IBM 24 Hours of Science, September, 20, 2023.
16. GraphEx Workshop, MIT Endicott House, August 15-16, 2023.
17. IAIFI Summer Workshop, Northeastern University, August 14–18, 2023 (video).
18. ICML Workshop on TAG-ML, Honolulu, HI, July 28th, 2023. (video)
19. RSS Workshop on Symmetries in Robot Learning, July 10th, Daegu, Republic of Korea, July 10th, 2023. (video)

20. [Remote] ML4Materials, Workshop @ ICLR '23, Fully Virtual, Kigali Rwanda, May 4 and 5, 2023.
21. Boston Symmetry Day, Northeastern University, April 7, 2023.
22. Learning and Emergence in Molecular Systems, IPAM at UCLA, January 23-27, 2023. (video)

2022

23. [Remote] NeurIPS AI4Science Workshop, New Orleans, LA, December 2nd, 2022.
24. [Remote] Boston University Materials Day, October 14, 2022.
25. [Remote] CECAM Workshop on Charting large materials dataspaces, CECAM-FR-RA, Grenoble, France, October 10-12, 2022.
26. [Remote] Symposium on the Future of Computing Research, Early Career Roundtable, September 12, 2022. (video)
27. Barcelona Methods in Molecular Simulation and Machine Learning Workshop, Barcelona Biomedical Research Park, CompBioMed, Barcelona, Spain, July 14-16, 2022. (video)
28. Swiss Equivariant Learning Workshop, CO2 - EPFL, Lasanne, Switzerland, July 11-14, 2022.
29. Variational Learning for Quantum Matter, Bernoulli Workshop - EPFL, Lausanne, Switzerland, July 4-8, 2022.
30. NSF Workshop on the Foundations of Machine Learning and its Applications for Scientific Discovery in Physical and Biological Systems, Tyson's Corner, VA.
31. Large-Scale First Principles Atomistic Simulation: Recent Advances and New Challenges American Physical Society (APS) March Meeting, Chicago, IL.

2021

32. [Remote] ELLIS Machine Learning for Molecule Discovery Workshop, December 13, 2021.
33. [Remote] Special Session on Theoretical and Applied perspectives in Machine Learning, AMS Fall Western Sectional Meeting, October 23, 2021.
34. [Remote] Machine Learning Materials Science, ACS Fall Meeting, August 23, 2021.

2020

35. [Remote] Keynote for Applied Computational Sciences symposium (ACOS), Dutch Research Council (NWO), Eindhoven, Netherlands. (video)
36. [Remote] Panelist on Architecture Design at The Analytical Foundations of Deep Learning Hosted by CDTI and UC Berkeley. (videos: talk | discussion)
37. [Remote] Workshop on Equivariance and Data Augmentation, University of Pennsylvania, Philadelphia, PA. (video)
38. [Remote] AI/ML for ALS Synchrotron Science Innovation forum, LBNL, Berkeley, CA.
39. [Remote] 1st Workshop on Scientific-Driven Deep Learning (SciDL). (video)
40. CECAM-Lorentz workshop on Computing Complex Mechanical Systems, EPFL, Lausanne, Switzerland.

2019

41. From Passive to Active: Generative and Reinforcement Learning with Physics, Institute of Pure and Applied Mathematics (IPAM) at UCLA, Los Angeles, CA. (video)
42. Machine Learning for Quantum Matter, Nordita, Stockholm, Sweden.
43. CNMS User Meeting, Oak Ridge National Laboratory, Oak Ridge, TN.
44. MolKin 2019: Molecular Kinetics and Sampling, Design and Machine Learning, Freie Universität Berlin, Berlin, Germany,

45. Machine Learning in Materials Genome, Anargyrios and Korgialenios School of Spetses, Spetses, Greece.
46. Structure in the Micro-world, TGDA at Ohio State University, Columbus, OH
47. Foundational & Applied Data Science for Molecular and Materials Sci. & Eng., I-DISC at Lehigh University, Bethlehem, PA.
48. Machine Learning in Nonlinear Physics and Mechanics, American Physical Society (APS) March Meeting, Boston, MA.
49. Molecular and Electronic Structure Theory Meets Data Science Session, Society for Industrial and Applied Mathematics (SIAM) Comp. Science and Engineering Conference, Spokane, WA.

2018

50. Machine Learning for Molecules and Materials Workshop, Conference on Neural Information Processing Systems (NeurIPS), Montreal, Canada
51. ML4Science Workshop, LBNL, Berkeley, CA (Sept. 2018)

Invited Seminars

2025

1. Tufts Electrical and Computer Engineering Seminar, October 31, 2025.
2. Materials Science Seminar at Columbia University, January 24, 2025.

2024

3. GRASP on Robotics Seminar, University of Pennsylvania, Philadelphia, PA, November 1st, 2024.
4. Materials Science Seminar, Yale University, New Haven, CT, October 30th, 2024.
5. Simons Foundation's ML@Flatiron Seminar Series, New York, NY May 14, 2024.
6. Simons Center for Computational and Physical Chemistry, NYU, March 25, 2024.
7. BIDMAP Seminar, UC Berkeley, February 1, 2024.

2023

1. [Remote] Materials Project Seminar, December 14, 2023. (video)
2. Applied AI Speaker Series, Argonne National Laboratory, November 15, 2023.
3. AI in Science Seminar Series, University of Chicago, November 14, 2023.
4. [Remote] Seminar, ORIGINS Data Science Lab (ODSL), Technical University in Munich, August 18, 2023.
5. MIT Numerical Methods for Partial Differential Equations Seminar, MIT, May 10, 2023.
6. AI Institute for Dynamic Systems Seminar, University of Washington, January 6th, 2023. (video)

2022

7. *[Remote]* AI4Science Seminar, Chalmers University of Technology, December 8th, 2022.
8. *[Remote]* Warwick Centre for Predictive Modelling, University of Warwick, October 3, 2022.
9. *[Remote]* Physics-informed machine learning seminar series, Los Alamos National Laboratory, September 29, 2022.
10. Physics Colloquium, McGill University, Montreal, Canada (February 25, 2022)

2021

11. *[Remote]* Leuven.AI Seminar at KU Leuven (October 7th, 2021)
12. *[Remote]* AI in Physics Seminar at Carnegie Mellon University (March 31, 2021)

13. *[Remote]* Cal State Los Angeles Physics Colloquium (March 25, 2021)
14. *[Remote]* MIT EECS Department Seminar (February 25, 2021)
15. *[Remote]* UC Berkeley Chemical and Biomolecular Engineering Department Seminar

2020

16. *[Remote]* Physics ∩ ML. (video)
17. *[Remote]* FHI Berlin, Berlin, Germany.
18. *[Remote]* Applied Artificial Intelligence Institute (AAII), UC Santa Cruz, Santa Cruz, CA.
19. Center for Computing Research, Sandia National Laboratories, Albuquerque, NM.

2019

20. eScience Institute at the University of Washington, Seattle, WA. (video)
21. Center for Computational Quantum Physics, Flatiron Institute, New York, NY.
22. Deep Learning Group, Sandia National Laboratories, Livermore, CA.

2018

23. Berkeley Statistics and Machine Learning Discussion Group, UC Berkeley, Berkeley, CA.
24. *Molecular Foundry,* LBNL, Berkeley, CA.

Invited Cross-sector Forums Talks

2025

1. Physics for future, University of Luxembourg, May 13-14

2024

2. Hudson Forum, IBM Thomas J. Watson Research Center, Yorktown Heights, NY, September 10

Contributed Talks

2021 - Machine Learning for Quantum Matter III, APS March Meeting.
2020 - *AI & Molecular World Track,* Applied ML Days, EPFL, Lausanne, Switzerland. (video)
2017 - *Computational Discovery and Design of Novel Materials Session,* APS March Meeting.
2016 - Comp. Materials Discovery & Design - Electronic Structure Sess., APS March Meeting.
2015 - *Focus Session: Honeycomb and Pyrochlore Lattices*, APS March Meeting.
2014 - *Focus Session: Frustrated Magnets and Spin-Orbit Coupling,* APS March Meeting.
2012 - *Accelerator Neutrino Experiments Session,* APS April Meeting.

Refereed Publications

1. *A Tale of Two Symmetries: Exploring the Loss Landscape of Equivariant Models,* YuQing Xie and Tess Smidt, NeurIPS (2025). OpenReview
2. *Training a Foundation Model for Materials on a Budget*, T. Koker, M. Kotak, and T. Smidt, AI for Accelerated Materials Design @ NeurIPS (2025). OpenReview
3. *Implicit Augmentation from Distributional Symmetry in Turbulence Super-Resolution*, J. Balla, J. Bailey, A. Backour, E. Hofgard, T. Jaakkola, T. Smidt, and R. McConkey, Machine Learning and the Physical Sciences Workshop @ NeurIPS 2025. OpenReview
4. *Accelerating Protein Molecular Dynamics Simulation with DeepJump*, A. D. S. Costa, M. Ponnapati, D. Rubin, T. Smidt, and J. Jacobson, AI for Science Workshop @ NeurIPS 2025. OpenReview

5. *EquiJump: Protein Dynamics Simulation via SO(3)-Equivariant Stochastic Interpolants*, A. D. S. Costa, I. Mitnikov, F. Pellegrini, A. Daigavane, M. Geiger, Z. Cao, K. Kreis, T. Smidt, E. Kucukbenli, and J. Jacobson, GEM Workshop @ ICLR 2025. OpenReview.
6. *The Price of Freedom: Exploring Tradeoffs between Expressivity and Computational Efficiency in* Equivariant Tensor Products, YuQing Xie, Ameya Daigavane, Mit Kotak, Tess Smidt, Accepted to ICML (2025) OpenReview and GRaM workshop at ICML (2024).
7. *EquiJump: Protein Dynamics Simulation via SO(3)-Equivariant Stochastic Interpolants,* Allan Dos Santos Costa, Ilan Mitnikov, Franco Pellegrini, Ameya Daigavane, Mario Geiger, Zhonglin Cao, Karsten Kreis, Tess Smidt, Emine Kucukbenli, Joseph Jacobsen, GEM Workshop @ ICLR (2024) OpenReview.
8. *Artificial intelligence for science in quantum, atomistic, and continuum systems,* Xuan Zhang, …. Tess Smidt, Shuiwang Ji, Foundations and Trends® in Machine Learning, 18(4), 385–912. (2025).
9. *Ligand-Mediated Quantum Yield Enhancement in 1-D Silver Organothiolate Metal–Organic Chalcogenolates,* M. Aleksich, Y. Cho, D. W. Paley, M. C. Willson, H. N. Nyiera, P. A. Kotei, V. Oklejas, D. W. Mittan- Moreau, E. A. Schriber, K. Christensen, I. Inoue, S. Owada, K. Tono, M. Sugahara, S. Inaba-Inoue, M. Vakili, C. J. Milne, F. DallAntonia, D. Khakhulin, F. Ardana-Lamas, F. Lima, J. Valerio, H. Han, T. Gallo, H. Yousef, O. Turkot, I. J. B. Macias, T. Kluyver, P. Schmidt, L. Gelisio, A. R. Round, Y. Jiang, D. Vinci, Y. Uemura, M. Kloos, A. P. Mancuso, M. Warren, N. K. Sauter, J. Zhao, T. Smidt, H. J. Kulik, S. Sharifzadeh, A. S. Brewster, J. N. Hohman, Adv. Funct. Mater., 2414914 (2024)
10. A Recipe for Charge Density Prediction, Xiang Fu, Andrew S. Rosen, Kyle Bystrom, Rui Wang, Albert Musaelian, Boris Kozinsky, Tess. Smidt, Tommi S. Jaakkola, NeurIPS (2024)
11. A Cosmic-Scale Benchmark for Symmetry-Preserving Data Processing, Julia Balla, Siddharth Mishra-Sharma, Carolina Cuesta-Lazaro, Tommi Jaakkola, Tess Smidt, LOG (2024) OpenReview
12. *Generalizing Denoising to Non-Equilibrium Structures Improves Equivariant Force Fields,* Yi-Lun Liao, Tess Smidt, Muhammed Shuaibi, Abhishek Das, TMLR (2024) OpenReview
13. *Equivariant Symmetry Breaking Sets,* YuQing Xie and Tess Smidt, TMLR (2024) OpenReview
14. *Discovering Symmetry Breaking in Physical Systems with Relaxed Group Convolution* Rui Wang, Elyssa Hofgard, Han Gao, Robin Walters, Tess Smidt, ICML (2024). OpenReview
15. *Quantifying Chemical Short-Range Order in Metallic Alloys,* Killian Sheriff, Yifan Cao, Tess Smidt, and Rodrigo Freitas, PNAS, 121 (25) e2322962121 (2024). DOI:10.1073/pnas.2322962121
16. *Ophiuchus: Scalable Modeling of Protein Structures through Hierarchical Coarse-graining SO(3)-Equivariant Autoencoders,* Allan dos Santos Costa, Ilan Mitnikov, Mario Geiger, Manvitha Ponnapati, Tess Smidt, Joseph Jacobson, ICLR Workshop on Generative and Experimental Perspectives for Biomolecular Design (GEM) (2024) OpenReview.
17. *EquiformerV2: Improved Equivariant Transformer for Scaling to Higher-Degree Representations,* Yi-Lun Liao, Brandon Wood, Abhishek Das, Tess Smidt, ICLR (2024) OpenReview
18. *Symphony: Symmetry-Equivariant Point-Centered Spherical Harmonics for Molecule Generation,* Ameya Daigavane, Song Kim, Mario Geiger, Tess Smidt, ICLR (2024). OpenReview

19. *Phonon predictions with E (3)-equivariant graph neural networks,* Shiang Fang, Mario Geiger, Joseph Checkelsky, Tess Smidt, AI for Accelerated Materials Design-NeurIPS Workshop (2023). OpenReview
20. *Relaxed Octahedral Group Convolution for Learning Symmetry Breaking in 3D Physical Systems,* Rui Wang, Robin Walters, Tess E. Smidt, AI4Science-NeurIPS Workshop (2023). OpenReview
21. *A Recipe for Cracking the Quantum Scaling Limit with Machine Learned Electron Densities,* Joshua A. Rackers, Lucas Tecot, Mario Geiger, Tess E. Smidt, Machine Learning: Science and Technology 4 015027 (2023). DOI 10.1088/2632-2153/acb314
22. *Equiformer: Equivariant Graph Attention Transformer for 3D Atomistic Graphs,* Yi-Lun Liao, Tess Smidt, ICLR (2023). arXiv:2206.11990
23. *Sign and Basis Invariant Networks for Spectral Graph Representation Learning,* Derek Lim, Joshua Robinson, Lingxiao Zhao, Tess Smidt, Suvrit Sra, Haggai Maron, Stefanie Jegelka ICLR (2023). arXiv:2202.13013
24. *Deep Learning and Spectral Embedding for Graph Partitioning,* A. Gatti, Z. Hu, T. Smidt, E. G. Ng, and P. Ghysels, Proceedings of the SIAM Conference on Parallel Processing for Scientific Computing (2022). DOI:10.1137/1.9781611977141.3
25. *Learning Integrable Dynamics with Action-Angle Networks,* Ameya Daigavane, Arthur Kosmala, Miles Cranmer, Tess Smidt, Shirley Ho, Workshop on Machine Learning in the Physical Sciences at NeurIPS (2022).
26. *Graph Partitioning and Sparse Matrix Ordering using Reinforcement Learning and Graph Neural Networks,* Alice Gatti, Zhixiong Hu, Tess Smidt, Esmond G. Ng, Pieter Ghysels, JMLR 23(303), (2022) arXiv:2104.03546
27. *Generative Coarse-Graining of Molecular Conformations,* Wujie Wang, Minkai Xu, Chen Cai, Benjamin Kurt Miller, Tess Smidt, Yusu Wang, Jian Tang, Rafael Gómez-Bombarelli, ICML (2022). arXiv:2201.12176
28. *E(3)-Equivariant Graph Neural Networks for Data-Efficient and Accurate Interatomic Potentials,* S. Batzner, A. Musaelian, L. Sun, M. Geiger, J. P. Mailoa, M. Kornbluth, N. Molinari, Tess Smidt and B. Kozinsky, Nature Communications 13, Article number: 2453 (2022). DOI:10.1038/s41467-022-29939-5
29. *SE(3)-equivariant prediction of molecular wavefunctions and electronic densities,* Oliver T. Unke, Mihail Bogojeski, Michael Gastegger, Mario Geiger, Tess Smidt, Klaus-Robert Müller *NeurIPS* (2021). arXiv:2106.02347
30. *Machine learning on neutron and x-ray scattering and spectroscopies,* Zhantao Chen, Nina Andrejevic, Nathan Drucker, Thanh Nguyen, R Patrick Xian, Tess Smidt, Yao Wang, Ralph Ernstorfer, Alan Tennant, Maria Chan, Mingda Li, Chemical Physics Reviews (Vol.2, Issue 3) (2021). DOI: 10.1063/5.0049111, *Highlight: How machine learning can augment neutron and X-ray scattering*, Meeri Kim. DOI: 10.1063/10.0005619
31. *Direct prediction of phonon density of states with Euclidean neural network*, Z. Chen*, N. Andrejevic*, **T. Smidt***, Z. Ding, Y. Chi, Q. T. Nguyen, A. Alatas, J. Kong, M. Li, Advanced Science, 2004214 (2021). arXiv:2009.05163 **denotes equal contribution*
32. *Finding symmetry breaking order parameters with Euclidean Neural Networks*, **T. Smidt**, M. Geiger, B. K. Miller, Physical Review Research 3, L012002 (2021). arXiv:2007.02005

33. *Euclidean Symmetry and Equivariance in Machine Learning*, **T. Smidt**, Trends in Chemistry, Volume 3, Issue 2, Pages 82-85 (2021). DOI:10.1016/j.trechm.2020.10.006
34. *Relevance of Rotationally Equivariant Convolutions for Predicting Molecular Properties*, B.K. Miller, M. Geiger, **T. Smidt,** and F. Noé, Accepted to ML4Molecules Workshop and Interpretable Inductive Biases and Physically Structured Learning Workshop, NeurIPS (2020). arXiv:2008.08461
35. *Anisotropic 2D Excitons Unveiled in Organic-Inorganic Quantum Wells,* Maserati, L. et al., Materials Horizons (2020). DOI:10.1039/C9MH01917K
36. *An Automatically Curated First-Principles Database of Ferroelectrics,* **T. Smidt**, S. A. Mack, S. Reyes-Lillo, A. Jain, J. B. Neaton, Scientific Data, 7, 72 (2020). DOI:10.1038/s41597-020-0407-9
37. *Atomate: A High-Level Interface to Generate, Execute, and Analyze Computational Materials Science Workflows*, Kiran Mathew et al., Comp. Mat. Science, Vol. 139, 140-152 (2017). DOI:10.1016/j.commatsci.2017.07.030
38. *Realization of a three-dimensional spin-anisotropic harmonic honeycomb iridate*, K. Modic, **T. Smidt,** et al., Nature Communications 5 (2014). DOI:10.1038/ncomms5203
39. *Testing of Cryogenic Photomultiplier Tubes for the MicroBooNE Experiment*, T. Briese et al., Journal of Instrumentation 8, T07005 (2013). arXiv:1304.0821,
40. *Proposal for an electron antineutrino disappearance search using high-rate 8Li production and decay,* A. Bungau et al. Physical Review Letters 109, 141802 (2012). arXiv:1205.4419
41. *Demonstration of a Lightguide Detector for Liquid Argon TPCs*, L. Bugel et al., Nuclear Instruments and Methods in Physics Research Section A (2011). arXiv:1101.3013

Preprints

1. *Phonon predictions with E(3)-equivariant graph neural networks,* Shiang Fang, Mario Geiger, Joseph G. Checkelsky, Tess Smidt (2024) arXiv:2403.11347
2. *Artificial intelligence for science in quantum, atomistic, and continuum systems,* Xuan Zhang, Limei Wang, Jacob Helwig, Youzhi Luo, Cong Fu, Yaochen Xie, Meng Liu, Yuchao Lin, Zhao Xu, Keqiang Yan, Keir Adams, Maurice Weiler, Xiner Li, Tianfan Fu, Yucheng Wang, Haiyang Yu, YuQing Xie, Xiang Fu, Alex Strasser, Shenglong Xu, Yi Liu, Yuanqi Du, Alexandra Saxton, Hongyi Ling, Hannah Lawrence, Hannes Stärk, Shurui Gui, Carl Edwards, Nicholas Gao, Adriana Ladera, Tailin Wu, Elyssa F Hofgard, Aria Mansouri Tehrani, Rui Wang, Ameya Daigavane, Montgomery Bohde, Jerry Kurtin, Qian Huang, Tuong Phung, Minkai Xu, Chaitanya K Joshi, Simon V Mathis, Kamyar Azizzadenesheli, Ada Fang, Alán Aspuru-Guzik, Erik Bekkers, Michael Bronstein, Marinka Zitnik, Anima Anandkumar, Stefano Ermon, Pietro Liò, Rose Yu, Stephan Günnemann, Jure Leskovec, Heng Ji, Jimeng Sun, Regina Barzilay, Tommi Jaakkola, Connor W Coley, Xiaoning Qian, Xiaofeng Qian, Tess Smidt, Shuiwang Ji (2023). arXiv:2307.08423
3. *e3nn: Euclidean Neural Networks,* Mario Geiger and Tess Smidt (2022). arXiv:2207.09453
4. *Tensor field networks: Translation- and 3D rotation-equivariant convolutional neural networks,* N. Thomas*, **T. Smidt***, S. Kearnes, L. Yang, L. Li, K. Kohlhoff, P. Riley, (2018). arXiv:1802.08219 **denotes equal contribution* **(Foundational paper for Euclidean neural networks, 450+ citations according to Google Scholar)**

Miscellaneous Publications

1. *[Patent] Mithrene and methods of fabrication of mithrene*, J.N. Hohman, M. Collins, and **T. Smidt**, U.S. Patent No. 10875828. Granted December 29, 2020. Filed August 4, 2017.
2. *[Conference proceedings] Simulations of Pion Production in the DAEδALUS Target*, A. Bungau, **T. Smidt** et al., International Particle Accelerator Conference (2012). arXiv:1205.5528
3. *[Whitepaper] Expression of Interest for a Novel Search for CP Violation in the Neutrino Sector: DAEdALUS*, J. Alonso et al., (2010). arXiv:1006.0260

Teaching

Courses

- Spring 2024: Instructor, 6.S966/8.S301 Symmetry and its Application to ML (60 students), MIT.
- Spring 2023: Instructor, 6.S966/8.S301 Symmetry and its Application to ML (44 students), MIT.
- Spring 2022: Co-lecturer, 6.730 Introduction to Solid State with Applications (20 students), MIT.
- Fall 2021/22: Instructor, 6.036 Introduction to Machine Learning (430 students), MIT.
- Spring 2011: Teaching assistant, 8.13 Junior Lab, MIT.
- Fall 2010: Teaching assistant, 8.01 Introduction to Classical Mechanics, MIT.

Guest Lectures

- [Remote] Lecture at UChicago AI+Science Summer School, July 15-19, 2024.
- Guest Lecture 6.S898 Deep Learning, MIT, October 3, 2023.
- Lecture for Summer Geometry Initiative, MIT, August 3, 2023.
- *[Remote]* Guest Lecture for 3.100J Machine Learning for Molecular Eng. at MIT, May 17, 2021.

Tutorials

2021

- *Tutorial on Symmetry Equivariant Neural Networks,* Material Research Society Fall Meeting
- *Lecture and Tutorial and E(3) Equivariant Neural Networks,* Bigmax Summer School

2020

- *E(3) Equivariant Neural Networks Tutorial,* Machine learning in Physics, Chemistry and Materials discussion group (MLDG), University of Cambridge, Cambridge, UK.
- *E(3) Equivariant Neural Networks Tutorial,* Scientific Machine Learning Mini-Course, Carnegie-Mellon University, Pittsburgh, PA.
- *Symmetry and Equivariance in Neural Networks,* Berkeley Lab Deep Learning School, LBNL, Berkeley, CA. (video)

2019 - *E(3) Equivariant Neural Networks Tutorial*, IPAM at UCLA, Los Angeles, CA.

Software

- Co-lead developer of *e3nn: A modular framework for Euclidean neural networks* https://github.com/e3nn/e3nn | *https://e3nn.org* | *https://docs.e3nn.org* 2019 - Present

Training

- *UCSF Scientific Leadership and Management Skills Course*, Gladstone Institute at UCSF, San Francisco, CA (May 1 and 8, 2019)

16 hours of training based on the HHMI publication Making the Right Moves: A Practical Guide to Scientific Management for Postdocs and New Faculty.

Outreach

- Catalyst Conversations: Atoms. Geometry. Algorithms. (video) December 15, 2023
- Midday Science Cafe, LBNL and UC Berkeley (video) May 20, 2021
- Skype a Scientist Fall 2020
- LBL Computing Sciences Summer Student Series, LBNL, Berkeley, CA 2019, 2020
- Penpal for Letters to a Pre-scientist 2018
- Seminar for Computational Materials at Berkeley, University of California, Berkeley, CA 2018

Advisees and Mentees (Students and Postdocs)

- *Ryley McConkey,* Postdoctoral Fellow, MIT RLE Fall 2024 - Current
- *Jigyasa Nigam*, Postdoctoral Fellow, MIT RLE Fall 2024 - Current
- *Teddy Koker,* PhD Student, MIT EECS Fall 2024 - Current
- *Giulianna Hashemi-Asasi,* PhD Student, MIT EECS Fall 2023 - Current
- *Mit Kotak,* SM Student, MIT CSE Fall 2023 - Current
- *Julia Balla,* PhD Student, MIT EECS Fall 2023 - Current
- *Max Aalto,* PhD Student, MIT EECS Fall 2023 - Current
- *Aria Mansouri Tehrani,* Postdoctoral Fellow, MIT RLE Spring 2023 - Current
- *Tuong Phung*, Undergraduate Student, MIT EECS Spring 2023 - Current
- *YuQing Xie*, PhD Student MIT EECS Fall 2022 - Current
- *Elyssa Hofgard*, PhD Student, MIT EECS Fall 2022 - Current
- *Ameya Daigavane*, PhD Student, MIT EECS Fall 2022 - Current
- *Adriana Ladera*, PhD Student, MIT CSE Fall 2022 - Current
- *Mario Geiger,* Postdoctoral Fellow, MIT RLE Spring 2022 - Summer 2023
- *Song Kim*, Undergraduate Student, MIT EECS Spring 2022 - Current
- *Yi-Lun Liao,* PhD Student, MIT EECS Fall 2021 - Current
- *Claire West*, PhD student at UW and Intern at LBNL Summer 2020
- *Elliott Perryman*, Undergrad the UT Knoxville and Intern at LBNL Spring 2020
- *Kostiantyn Lapchevskyi*, MA student at Ukrainian Catholic University Fall 2019
  - Advised Master's thesis:
  - *"Predicting Properties of Crystals"*
- *Simon Batzner*, SM student at MIT and PhD student at Harvard Fall 2019
  - Provided mentorship during Master's thesis:
  - *"Learning symmetry-preserving interatomic force fields for atomistic simulations"*
- *Mario Geiger,* PhD student at EPFL and Intern at LBNL Summer 2019
- *Benjamin K. Miller*, MA student at FU Berlin and Intern at LBNL Summer 2019
  - Provided mentorship during Master's thesis:
  - "SE(3) Equivariant Neural Networks for Regression on Molecular Properties"
  - Currently a PhD student at the AMLab at University of Amsterdam.
- *Hashim Piracha*, BS student at UC Berkeley and Intern at LBNL Summer 2019

Professional Service

- *Co-organizer of Bay Area Scientific Computing Day*, LBNL, Berkeley, CA (2019)
- Machine Learning and Analytics Group Lead Search Committee, LBNL, Berkeley, CA (2021)
- Symposium co-organizer, Materials Research Society Fall Meeting (2021)
- MIT EECS PhD Program Admissions Committee (2021, 2022, 2023)
- MIT CSE SM Program Admissions Committee (2021, 2022, 2023)
- Co-organizer of the *Swiss Equivariant Learning Workshop*, EPFL, Lausanne, Switzerland (2022)
- MIT Path of Professorship Workshop – Session: Negotiating the Offer, November 19th (2022).
- MIT Hobby Shop Committee (2022 to present).
- Regular Member, Committee to design new CSE PhD program (2022-2023)
- Co-organizer, Rising Stars in EECS Academic Career Workshop (2024).
- NSF Inst. of AI and Fundamental Interactions Committees: Steering Committee (2022 - present), Summer Workshop (2022), Renewal Committee (2023), Equity and Early Career Committee (2023), Fellowship Committee (2024), Fellowship Committee (2025)

Mischief

- **Woodworking** – Active member of the MIT Hobby Shop. Recent projects: Lasagna Noodle Desk made of Maple, Ladder, 3D Tetris Ottomans
- **Pole Dancing & Aerial Arts** – 1st place, Hardstyle Level 3 at Pole Sport Organization Northeast 2024. Intensive Program training in Chinese Pole Fall I & II 2025 at the New England Center for Circus Arts (NECCA). Trains regularly in pole and other aerial arts for physical expression and structured defiance of gravity.
- ***Modeling Matter(s)*** -- A podcast that showcased early career researchers and the mental models they use to investigate the world around us. (Fall 2020 - Spring 2021, on hiatus)
- ***The Lunch Experiment*** -- Developed an automated system that invited grad students from different departments to group lunches. Organized over 150 "randomized controlled lunches" and grew a community of more than 400 grad students from 50 departments. (Summer 2015 - Spring 2016)
- ***Cosmic Ray Chandeliers*** -- Funded by MIT to design, fabricate, and install two 4' tall chandeliers that illuminate upon detecting cosmic ray muons – particles created when nuclei from outer space bombard Earth's atmosphere. Located on the 5th floor of building 26. (Spring 2011)
- ***blondegeek.net*** -- Launched t-shirt company in Summer 2006 at age 16. Designed website, created customer and product databases and wrote inventory management software. During ten years of business, designed and sold thousands of shirts. (2006-2016)
- **Weightlifting** -- (in gym PRs) SQ: 1.7 x BW, BP: 0.9 x BW, DL: 2.5 x BW