

Tess Eleonora Smidt

Curriculum Vitae

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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 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

Assistant Professor, Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology 2021 - present

Luis W. Alvarez Postdoctoral Fellow, Lawrence Berkeley National Laboratory 2018 - 2021
Designing symmetry-preserving neural networks for applications across the physical sciences such as: generating 3D point geometries, ab initio molecular dynamics, and crystal property prediction. Creating new algorithms that exploit the properties of symmetry-preserving neural networks. 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). Created machine learning models for heterogeneous catalysis.

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

<u>Rising Stars in Computational and Data Science</u> , Oden Institute at UT Austin	2019
People's Choice Winner, Lawrence Berkeley National Laboratory Research SLAM (video)	2019
<u>Luis W. Alvarez Postdoctoral Fellowship</u> , Lawrence Berkeley National Laboratory	2018
National Science Foundation Research Fellowship	2012

Invited Conference and Workshop Talks

2022

- NSF Workshop on the Foundations of Machine Learning and its Applications for Scientific Discovery in Physical and Biological Systems, Tyson's Corner, VA.
- Large-Scale First Principles Atomistic Simulation: Recent Advances and New Challenges American Physical Society (APS) March Meeting, Chicago, IL.

2021

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

2020

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

2019

- From Passive to Active: Generative and Reinforcement Learning with Physics, Institute of Pure and Applied Mathematics (IPAM) at UCLA, Los Angeles, CA. ([video](#))
- Machine Learning for Quantum Matter, Nordita, Stockholm, Sweden.
- CNMS User Meeting, Oak Ridge National Laboratory, Oak Ridge, TN.
- MolKin 2019: Molecular Kinetics and Sampling, Design and Machine Learning, Freie Universität Berlin, Berlin, Germany,
- Machine Learning in Materials Genome, Anargyrios and Korgialenios School of Spetses, Spetses, Greece.
- Structure in the Micro-world, TGDA at Ohio State University, Columbus, OH
- Foundational & Applied Data Science for Molecular and Materials Sci. & Eng., I-DISC at Lehigh University, Bethlehem, PA.
- Machine Learning in Nonlinear Physics and Mechanics, American Physical Society (APS) March Meeting, Boston, MA.

- *Molecular and Electronic Structure Theory Meets Data Science Session*, Society for Industrial and Applied Mathematics (SIAM) Comp. Science and Engineering Conference, Spokane, WA.

2018

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

Invited Seminars

2022

- Physics Colloquium, McGill University, Montreal, Canada (February 25, 2022)

2021

- [Remote] Leuven.AI Seminar at KU Leuven (October 7th, 2021)
- [Remote] Guest Lecture for 3.100J Machine Learning for Molecular Eng. at MIT (May 17, 2021)
- [Remote] AI in Physics Seminar at Carnegie Mellon University (March 31, 2021)
- [Remote] Cal State Los Angeles Physics Colloquium (March 25, 2021)
- [Remote] MIT EECS Department Seminar (February 25, 2021)
- [Remote] UC Berkeley Chemical and Biomolecular Engineering Department Seminar

2020

- [Remote] *Physics \cap ML*. ([video](#))
- [Remote] FHI Berlin, Berlin, Germany.
- [Remote] Applied Artificial Intelligence Institute (AAIL), UC Santa Cruz, Santa Cruz, CA.
- Center for Computing Research, Sandia National Laboratories, Albuquerque, NM.

2019

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

2018

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

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

*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](#)

SE(3)-Equivariant Graph Neural Networks for Data-Efficient and Accurate Interatomic Potentials

Simon Batzner, Tess E. Smidt, Lixin Sun, Jonathan P. Mailoa, Mordechai Kornbluth, Nicola Molinari, Boris Kozinsky, Nature Communications 13, Article number: 2453 (2022). [arXiv:2101.03164](https://arxiv.org/abs/2101.03164)

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](https://arxiv.org/abs/2106.02347)

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](https://doi.org/10.1063/5.0049111)

Highlight: How machine learning can augment neutron and X-ray scattering, Meeri Kim.

[DOI: 10.1063/10.0005619](https://doi.org/10.1063/10.0005619)

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](https://doi.org/10.1002/advs.2004214) (2021). [arXiv:2009.05163](https://arxiv.org/abs/2009.05163) *denotes equal contribution

Finding symmetry breaking order parameters with Euclidean Neural Networks

T. Smidt, M. Geiger, B. K. Miller, Physical Review Research 3, [L012002](https://doi.org/10.1103/PhysRevResearch.3.012002) (2021). [arXiv:2007.02005](https://arxiv.org/abs/2007.02005)

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](https://doi.org/10.1016/j.trechm.2020.10.006)

Relevance of Rotationally Equivariant Convolutions for Predicting Molecular Properties

B.K. Miller, M. Geiger, **T. Smidt**, and F. Noé, Accepted to [ML4Molecules Workshop](https://www.molssi.org/workshop/) and [Interpretable Inductive Biases and Physically Structured Learning Workshop](https://www.molssi.org/workshop/), *NeurIPS* (2020). [arXiv:2008.08461](https://arxiv.org/abs/2008.08461)

Anisotropic 2D Excitons Unveiled in Organic-Inorganic Quantum Wells

Maserati, L. et al., Materials Horizons (2020).

[DOI:10.1039/C9MH01917K](https://doi.org/10.1039/C9MH01917K)

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](https://doi.org/10.1038/s41597-020-0407-9)

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](https://doi.org/10.1016/j.commatsci.2017.07.030)

Realization of a three-dimensional spin-anisotropic harmonic honeycomb iridate

K. Modic, **T. Smidt**, et al., Nature Communications 5 (2014).

[DOI:10.1038/ncomms5203](https://doi.org/10.1038/ncomms5203)

Testing of Cryogenic Photomultiplier Tubes for the MicroBooNE Experiment

T. Briese et al., Journal of Instrumentation 8, T07005 (2013). [arXiv:1304.0821](https://arxiv.org/abs/1304.0821)

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](https://arxiv.org/abs/1205.4419)

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](https://arxiv.org/abs/1101.3013)

Preprints

Equiformer: Equivariant Graph Attention Transformer for 3D Atomistic Graphs

Yi-Lun Liao, Tess Smidt (2022). [arXiv:2206.11990](https://arxiv.org/abs/2206.11990)

Sign and Basis Invariant Networks for Spectral Graph Representation Learning

Derek Lim, Joshua Robinson, Lingxiao Zhao, Tess Smidt, Suvrit Sra, Haggai Maron, Stefanie Jegelka (2022). [arXiv:2202.13013](https://arxiv.org/abs/2202.13013)

Cracking the Quantum Scaling Limit with Machine Learned Electron Densities

Joshua A. Rackers, Lucas Tecot, Mario Geiger, Tess E. Smidt (2022). [arXiv:2201.03726](https://arxiv.org/abs/2201.03726)

Deep Learning and Spectral Embedding for Graph Partitioning

Alice Gatti, Zhixiong Hu, Tess Smidt, Esmond G. Ng, Pieter Ghysels (2021). [arXiv:2110.08614](https://arxiv.org/abs/2110.08614)

Graph Partitioning and Sparse Matrix Ordering using Reinforcement Learning

Alice Gatti, Zhixiong Hu, Tess Smidt, Esmond G. Ng, Pieter Ghysels (2021). [arXiv:2104.03546](https://arxiv.org/abs/2104.03546)

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](https://arxiv.org/abs/1802.08219)

*denotes equal contribution

(Foundational paper for Euclidean neural networks, 300+ citations according to Google Scholar)

Miscellaneous Publications

[Patent] Mithrene and methods of fabrication of mithrene

J.N. Hohman, M. Collins, and **T. Smidt**

[U.S. Patent No. 10875828](https://patent.google.com/patent/US10875828). Granted December 29, 2020. Filed August 4, 2017.

[Conference proceedings] Simulations of Pion Production in the DAE δ ALUS Target

A. Bungau, **T. Smidt** et al., International Particle Accelerator Conference (2012). [arXiv:1205.5528](https://arxiv.org/abs/1205.5528)

[Whitepaper] *Expression of Interest for a Novel Search for CP Violation in the Neutrino Sector: DAEdALUS*

J. Alonso et al., (2010). [arXiv:1006.0260](https://arxiv.org/abs/1006.0260)

Grants

2021

- [DE-FOA-0002482](#): DOE Integrated Computational and Data Infrastructure for Science. AI Tools for the Characterization and Design of Achievable Hypothetical Materials. [Press Release](#).

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.

Teaching

- Spring 2022: Co-lecturer, 6.730 Introduction to Solid State with Applications (20 students), MIT.
- Fall 2021: 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.

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

- [Midday Science Cafe](#), LBNL and UC Berkeley ([video](#)) May 20, 2021

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- *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

Advised and Mentored Students and Postdocs

- *Mario Geiger*, Postdoctoral Fellow, MIT RLE 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 (2022)
- MIT CSE SM Program Admissions Committee (2022)
- Co-organizer of the *Swiss Equivariant Learning Workshop*, EPFL, Lausanne, Switzerland (2022)

Mischief

- [Modeling Matter\(s\)](#) -- A podcast that showcases early career researchers and the mental models they use to investigate the world around us. (Fall 2020 - present)
- [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