

Tess Eleonora Smidt

Curriculum Vitae

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Research Interests

Neural networks from first-principles for rich datatypes (e.g. scientific data and geometry), chemical and material science and design, group theory and symmetry, scientific computing, density functional theory, computational geometry, Euclidean Neural Networks.

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

Luis W. Alvarez Postdoctoral Fellow, Lawrence Berkeley National Laboratory 2018 - present
Designing symmetry-preserving neural networks for applications across the physical sciences (e.g. generating 3D point geometries, ab initio molecular dynamics, crystal property prediction). Creating new algorithms that exploit the properties of symmetry-preserving neural networks (e.g. finding symmetry implied missing data without using conventional symmetry analysis). Developer of `e3nn`: an open-source modular PyTorch framework for Euclidean neural networks.

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 learned 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.

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 the new neutrino source for IsoDAR. 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. Developed scalable and efficient method for fabricating acrylic lightguides to enable light detection in kiloton neutrino detectors.

Awards

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

Invited Conference and Workshop Talks (Upcoming and Previous)

2020

- *[Remote] Keynote for Applied Computational Sciences symposium (ACOS)*, Dutch Research Council (NWO), Eindhoven, Netherlands.
- *[Remote] Workshop on Equivariance and Data Augmentation*, University of Pennsylvania, Philadelphia, PA.
- *[Remote] AI/ML for ALS Synchrotron Science Innovation forum*, LBNL, Berkeley, CA.
- *[Remote] [1st Workshop on Scientific-Driven Deep Learning \(SciDL\)](https://scidl.netlify.app/)* (<https://scidl.netlify.app/>).
- *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.
- *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 (Upcoming and Previous)

2020

- [Remote] [Physics \$\cap\$ ML](http://physicsmeetsml.org/) (physicsmeetsml.org/).
- [Remote] FHI Berlin, Berlin, Germany.
- [Remote] Applied Artificial Intelligence Institute (AAII), 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.
- 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 (Upcoming and Previous)

2020 - *AI & Molecular World Track*, Applied ML Days, EPFL, Lausanne, Switzerland

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, Atlanta, GA

Refereed Publications

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](https://arxiv.org/abs/2008.08461)

Euclidean Symmetry and Equivariance in Machine Learning,

T. Smidt, In press, Trends in Chemistry, Month 2020, Vol. xx, No. xx (2020).

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

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).

*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).

Realization of a three-dimensional spin-anisotropic harmonic honeycomb iridate
K. Modic, **T. Smidt**, et al., Nature Communications 5 (2014). [arXiv:1402.3254](https://arxiv.org/abs/1402.3254)

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

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,
Submitted (2020). [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, Submitted (2020). [arXiv:2007.02005](https://arxiv.org/abs/2007.02005)

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, 100+ citations according to Google Scholar)

Miscellaneous Publications

[Pending patent] Mithrene and methods of fabrication of mithrene
J.N. Hohman, M. Collins, and **T. Smidt**.

International Patent App. PCT/US2017/045609. Filed August 4, 2017. Published as [US20190194128A1](#) June 27, 2019.

[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](#)

[Whitepaper] *Expression of Interest for a Novel Search for CP Violation in the Neutrino Sector: DAE δ ALUS*
J. Alonso et al., (2010). [arXiv:1006.0260](#)

Software

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

Tutorials / Teaching

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.

2019 - [E\(3\) Equivariant Neural Networks Tutorial](#), IPAM at UCLA, Los Angeles, CA.

2011 - Teaching assistant, 8.13 Junior Lab, MIT.

2010 - Teaching assistant, 8.01 Introduction to Mechanics, MIT.

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

- *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, Berkeley, CA (2018)

Advised and Mentored Students

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- *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

Collaborators

- Prof. Boris Kozinsky, Harvard University
- Prof. Mingda Li, Massachusetts Institute of Technology
- Prof. Frank Noé, Freie Universität Berlin
- Dr. Josh Rackers, Sandia National Laboratories
- Dr. Thomas Hardin, Sandia National Laboratories
- Dr. Eugene Kwan, Merck
- Dr. Doug Tischer, University of Washington

Professional Service

- Co-organizer of [2019 Bay Area Scientific Computing Day](#), LBNL, Berkeley, CA (2019)

Mischief

- **Modeling Matter(s)** -- A podcast that showcases early career researchers and the mental models they use to investigate the world around us. <http://modelingmatters.com/> (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. <http://www.blondegeek.net/cosmicray/> (Fall 2010 - 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)