

TEDDY KOKER

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EDUCATION

- Massachusetts Institute of Technology** Sep. 2024 - Present
Ph.D. in Electrical Engineering and Computer Science
Advised by Prof. Tess Smidt
- Worcester Polytechnic Institute** Sep. 2016 - Dec. 2019
B.S. in Computer Science with Distinction

RESEARCH EXPERIENCE

- Massachusetts Institute of Technology** Sep. 2024 - Present
Research Assistant with Prof. Tess Smidt
- Massachusetts Institute of Technology, Lincoln Laboratory** Apr. 2021 - Aug. 2024
Associate Staff, AI Technology Group
- Created E(3) equivariant neural networks for electron density prediction in materials and organic molecules ([ChargE3Net](#)).
 - Developed methods for contrastive representation learning of crystalline materials with graph neural networks ([CrystalCLR](#)).
 - Researched domain adaptation and interpretability methods for timeseries models in collaboration with the Zitnik Lab at Harvard Medical School ([Raincoat](#), [TimeX](#)).
- Lightning AI** Aug. 2020 - Feb. 2021
Machine Learning Research Engineer
- Created a python library with efficient and scalable implementations of common machine learning evaluation metrics ([torchmetrics](#)).
 - Introduced a method of generating pixel level saliency maps for model interpretability ([U-Noise](#)).
 - Researched self-supervised learning of image representations with augmented autoencoders ([AASAE](#)).
- Harvard Medical School** Dec. 2019 - Aug. 2020
Research Associate, Image and Data Analysis Core
- Created deep learning model to detect manipulation of microscopy images, along with a new training and benchmark dataset ([BINDER](#)).

PUBLICATIONS

- T. Koker**, M. Kotak, T. Smidt. *Training a Foundation Model for Materials on a Budget*. NeurIPS AI for Accelerated Materials Discovery Workshop, 2025.
- T. Koker**, K. Quigley, E. Taw, K. Tibbetts, L. Li. *Higher-Order Equivariant Neural Networks for Charge Density Prediction in Materials*. npj Computational Materials, 2024. Also at NeurIPS AI4Science Workshop, 2023.
- S. Gao, **T. Koker**, O. Queen, T. Hartvigsen, T. Tsiligkaridis, M. Zitnik. *UniTS: Building a Unified Time Series Model*. NeurIPS, 2024.
- O. Queen, T. Hartvigsen, **T. Koker**, H. He, T. Tsiligkaridis, M. Zitnik. *Encoding Time-Series Explanations through Self-Supervised Model Behavior Consistency*. NeurIPS, 2023.[†]

[†]Spotlight award, top 3% of submissions

- H. He, O. Queen, **T. Koker**, C. Cuevas, T. Tsiligkaridis, M. Zitnik. *Domain Adaptation for Time Series Under Feature and Label Shifts*. International Conference on Machine Learning (ICML), 2023.
- **T. Koker**, K. Quigley, W. Spaeth, N. C. Frey, L. Li. *Graph Contrastive Learning for Materials*. NeurIPS AI for Accelerated Materials Design Workshop, 2022.
- N. S. Detlefsen, J. Borovec, J. Schock, A. H. Jha, **T. Koker**, L. D. Liello, D. Stancl, C. Quan, M. Grechkin, W. Falcon. *TorchMetrics - Measuring Reproducibility in PyTorch*. The Journal of Open Source Software (JOSS), 2022.
- W. Falcon, A. H. Jha, **T. Koker**, K. Cho. *AASAE: Augmentation-Augmented Stochastic Autoencoders*. arXiv, 2021.
- **T. Koker**, F. Mireshghallah, T. Titcombe, G. Kaissis. *U-Noise: Learnable Noise Masks for Interpretable Image Segmentation*. International Conference on Image Processing (ICIP), 2021.
- **T. Koker***, S. S. Chintapalli*, S. Wang, B. A. Talbot, D. Wainstock, M. Cicconet, M. C. Walsh. *On Identification and Retrieval of Near-Duplicate Biological Images: a New Dataset and Protocol*. International Conference on Pattern Recognition (ICPR), 2020.
- **T. Koker**, D. Koutmos. *Cryptocurrency Trading Using Machine Learning*. Journal of Risk and Financial Management, 2020.

HONORS & AWARDS

MIT

- NSF Graduate Research Fellowship (declined), 2025.
- Robert J. Shillman (1974) Fund Fellowship, 2024.

MIT Lincoln Laboratory

- Line Grant, 2023. Awarded \$295,000 for research on machine learning for medical decision-making. Co-PI with Keegan Quigley.
- Team Award, 2022. Highest group award at Lincoln Laboratory.

Worcester Polytechnic Institute

- Dean's List, 2017 - 2019. Distinguished academic performance.
- Global Scholarship, 2018. Awarded to defray cost of off-campus project.
- Charles O. Thompson Scholar, 2017. Outstanding performance by first year students.
- Presidential Scholarship, 2016 - 2019.

SERVICE & LEADERSHIP

Talks

- Speaker, ML-Driven Discovery Retreat at MIT. Sep. 2025
- Poster presenter, AI4Chemistry Summit at NYU. Jun. 2025
- Speaker, Graph Exploitation Symposium at MIT. Jul. 2024
- Poster presenter, Gordon Research Conference on Computational Materials Science. Jul. 2024
- Poster presenter, Graph Exploitation Symposium at MIT. Aug. 2023
- Speaker, Chemical and Biological Defense Science & Technology Conference. Dec. 2022
- Speaker, Recent Advances in AI for National Security at MIT Lincoln Laboratory. Nov. 2021

*Equal contribution

Volunteering

- Reviewing: NeurIPS, Nature Communications, npj Computational Materials, npj Digital Medicine.
- Research Lead, [OpenMined](#). Apr. 2020 - May 2021

SELECT PROJECTS

Personal Writing

- *Neural Variational Monte Carlo* Nov. 2024
- *Learning to Learn with JAX* Apr. 2022
- *Performers: The Kernel Trick, Fourier Features, and Attention* Dec. 2020
- *Deep Learning for Guitar Effect Emulation* May. 2020
- *NLP from Scratch: Annotated Attention* Feb. 2020

Software

- [torchsort](#). *700+ stars*. PyTorch library implementing the *Fast Differentiable Sorting and Ranking* algorithm, optimized with custom C++ and CUDA extensions.
- [torchmetrics](#). *1.6k+ stars*. Machine learning metrics for distributed and scalable PyTorch applications.