

# TEDDY KOKER

Cambridge, MA ◊ [tekoker@mit.edu](mailto:tekoker@mit.edu)  
[teddykoker.com](http://teddykoker.com) ◊ [github.com/teddykoker](https://github.com/teddykoker)

## EDUCATION

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

## RESEARCH EXPERIENCE

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<b>Massachusetts Institute of Technology</b> <i>Research Assistant with Prof. Tess Smidt</i>	Sep. 2024 - Present
<ul style="list-style-type: none"><li>Proposed phonon fine-tuning (<a href="#">PFT</a>), a method for training machine learned interatomic potentials (MLIPs) directly on phonon calculations for superior thermodynamic property prediction.</li><li>Introduced a recipe for training universal MLIPs with a small computational budget (<a href="#">Nequix</a>).</li></ul>	
<b>Massachusetts Institute of Technology, Lincoln Laboratory</b> <i>Associate Staff, AI Technology Group</i>	Apr. 2021 - Aug. 2024
<ul style="list-style-type: none"><li>Created E(3) equivariant neural networks for electron density prediction in materials and organic molecules (<a href="#">ChargE3Net</a>).</li><li>Developed methods for contrastive representation learning of crystalline materials with graph neural networks (<a href="#">CrystalCLR</a>).</li><li>Researched domain adaptation and interpretability methods for timeseries models in collaboration with the Zitnik Lab at Harvard Medical School (<a href="#">Raincoat</a>, <a href="#">TimeX</a>).</li></ul>	
<b>Lightning AI</b> <i>Machine Learning Research Engineer</i>	Aug. 2020 - Feb. 2021
<ul style="list-style-type: none"><li>Created a python library with efficient and scalable implementations of common machine learning evaluation metrics (<a href="#">torchmetrics</a>).</li><li>Introduced a method of generating pixel level saliency maps for model interpretability (<a href="#">U-Noise</a>).</li><li>Researched self-supervised learning of image representations with augmented autoencoders (<a href="#">AASAE</a>).</li></ul>	
<b>Harvard Medical School</b> <i>Research Associate, Image and Data Analysis Core</i>	Dec. 2019 - Aug. 2020
<ul style="list-style-type: none"><li>Created deep learning model to detect manipulation of microscopy images, along with a new training and benchmark dataset (<a href="#">BINDER</a>).</li></ul>	

## PUBLICATIONS

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- T. Koker**, A. Gangan, M. Kotak, J. Marian, T. Smidt. *PFT: Phonon Fine-tuning for Machine Learned Interatomic Potentials*. arXiv, 2026.
  - 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. Tsilgkaridis, M. Zitnik. *UniTS: Building a Unified Time Series Model*. NeurIPS, 2024.
- O. Queen, T. Hartvigsen, **T. Koker**, H. He, T. Tsilgkaridis, M. Zitnik. *Encoding Time-Series Explanations through Self-Supervised Model Behavior Consistency*. NeurIPS, 2023.<sup>†</sup>
- H. He, O. Queen, **T. Koker**, C. Cuevas, T. Tsilgkaridis, 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. Kaassis. *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

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### 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

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### Talks

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|--|-----------|
| · 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 |

<sup>†</sup>Spotlight award, top 3% of submissions

\*Equal contribution

- Speaker, Chemical and Biological Defense Science & Technology Conference. Dec. 2022
- Speaker, Recent Advances in AI for National Security at MIT Lincoln Laboratory. Nov. 2021

### Volunteering

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

## SELECT PROJECTS

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### 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.