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

- Proposed phonon fine-tuning (PFT), a method for training machine learned interatomic potentials (MLIPs) directly on phonon calculations for superior thermodynamic property prediction.
- Introduced a recipe for training universal MLIPs with a small computational budget (Nequix).

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**, 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. 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.†

· 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

†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

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.