

Donald Loveland

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EDUCATION

University of Michigan, Ann Arbor

2021–2026

Ph.D. in Computer Science

Ann Arbor, MI

- **Advisor:** Danai Koutra - Graph Exploration and Mining at Scale (GEMS) Lab
- **Fellowships:** Rackham Merit Fellow
- **Research Interests:** Explainability, Robustness, and Fairness applied to Graph Neural Networks.

California Polytechnic State University, San Luis Obispo

2014–2018

B.Sc. in Physics

San Luis Obispo, CA

- **Minors:** Computer Science, Mathematics, Astronomy, Ethnic Studies
- **GPA:** 3.61/4.00 (*Cum Laude*)

RECENT EXPERIENCE

Lawrence Livermore National Lab

Feb. 2019 - Sept. 2021

Staff Scientist - Applied Machine Learning Researcher

Livermore, CA

- Developed an explainable AI method for counterfactual introspection of DL models. Applied to materials science applications to extract domain-specific concepts learned by CNN models.
- Created an introspection and inverse design method for graph neural networks through reinforcement learning.
- Explored relationship between adversarial training and post-hoc explainable AI methods for GNNs. Demonstrated interplay between robustness and explainability.

Chevron

Aug. 2018 - Feb. 2019

Software Engineer

San Ramon, CA

- Developed a cloud deployment framework for ML models through Microsoft Azure.

SUBMITTED PRE-PRINTS

1. J. Zhu, J. Jin, **D. Loveland**, M. Schaub, D. Koutra, "On the Relationship Between Heterophily and Robustness of Graph Neural Network", *Submitted to The Tenth International Conference on Learning Representations (ICLR)*, 2022

SELECTED PUBLICATIONS (* denotes equal contribution)

1. **D. Loveland**, S. Liu, B. Kailkhura, A. Hiszpanski, Y. Han, "Reliable Graph Neural Network Explanations Through Adversarial Training", *ICML Workshop on Theoretic Foundation, Criticism, and Application Trend of Explainable AI*, 2021
2. P. Nguyen*, **D. Loveland***, J. Kim, P. Karande, A. M. Hiszpanski, Y. Han, "Predicting Energetics Materials Crystalline Density from Chemical Structure by Machine Learning", *Journal of Chemical Information and Modeling*, 2021
3. **D. Loveland**, B. Kailkhura, P. Karande, A. M. Hiszpanski, Y. Han, "Automated Identification of Molecular Crystals Packing Motifs", *Journal of Chemical Information and Modeling*, 2020
4. B. Gallagher, M. Rever, **D. Loveland**, T. N. Mundhenk, B. Beauchamp, et al, "Predicting Compressive Strength of Consolidated Molecular Solids using Computer Vision and Deep Learning", *Materials and Design*, 2020
5. S. Liu, B. Kailkhura, **D. Loveland**, Y. Han, "Generative Counterfactual Introspection for Explainable Deep Learning", *IEEE Global Conference on Signal and Information Processing (GlobalSIP)*, 2019