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**: Explainable AI (XAI), robustness, and fairness applied to graph neural networks (GNNs).

California Polytechnic State University, San Luis Obispo 2014 - 2018
B.S. in Physics (3.61/4.00 GPA) San Luis Obispo, CA

- **Minors**: Computer Science, Mathematics, Astronomy, Ethnic Studies

RECENT EXPERIENCE

Lawrence Livermore National Lab Feb. 2019 - Sept. 2021
Staff Scientist - Applied Machine Learning Researcher Livermore, CA

- Developed an XAI method for counterfactual introspection of DL models in PyTorch. Method was applied to materials science problems to extract domain-specific concepts learned by convolution neural networks. US patent pending.
- Explored the relationship between adversarial training and post-hoc XAI methods for GNNs in PyTorch Geometric. Findings were presented at ICML XAI Workshop and used to elucidate important molecular substructures.
- Created an inverse design method for molecular graphs through a GNN-based RL model. New molecules were designed through an interpretable graph editing policy. Work was used to aid scientists in molecule discovery tasks.

Chevron Aug. 2018 - Feb. 2019
Software Engineer San Ramon, CA

- Developed a cloud deployment pipeline for ML models through Microsoft Azure. Automation streamlined a multi-day manual process, reducing development time to a few hours. Won Chevron's Cloud Innovation Award for 2019.

SUBMITTED PREPRINTS UNDER REVIEW

- 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

- **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
- 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
- **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
- 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
- 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

*Denotes equal contribution