Donald Loveland

Email: dlovelan@umich.edu | **Website:** donaldloveland.com | **LinkedIn:** donald-loveland

RESEARCH INTERESTS

My work focuses on fundamental research in **graph representation learning** and **graph neural networks (GNNs)**. Specifically, I study how to improve the interpretability, robustness, and fairness of GNNs in real-world settings. I am currently investigating how heterophily (i.e., a tendency for dissimilar nodes to connect) impacts post-hoc explanations to develop new introspection techniques that leverage learned representations in an unbiased manner.

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

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

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

*Denotes equal contribution

- **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, J. Zhang, A. M. Hiszpanski, E. Robertson, **D. Loveland**, Y. Han. "Actionable attribution maps for scientific machine learning", *ICML Workshop on ML Interpretability for Scientific Discovery*, 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
- V. N. Bennert, **D. Loveland**, E. Donohue, M. Cosens, S. Lewis, et al, "Studying the [OIII]λ 5007Å emission-line width in a sample of 80 local active galaxies: a surrogate for σ*?", *Monthly Notices of the Royal Astronomical Society*, 2018

TALKS AND POSTERS

- Poster (virtual), *ICML Workshop on Theoretic Foundation, Criticism, and Application Trend of Explainable AI*, "Reliable Graph Neural Network Explanations Through Adversarial Training". 2021.
- Talk (virtual), *Materials Science and Technology*, “Automated Identification of Molecular Packing Motifs”. 2020.
- Talk, *Minerals, Metals and Materials*, “Automated Anomaly Detection in CT Scans”. 2020.
- Poster, *Materials Research Society*, “Comparison of Neural Network Based Models and Molecular Fingerprints for Density Prediction of Small Molecules”. 2019.
- Poster, *Materials Science and Technology*, “Predicting Compressive Strength of Consolidated Solids using Computer Vision and Deep Learning”. 2019.