Daniel Levy

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scholar.google.com/citations?user=Bcw9X7QAAAAJ

Machine Learning PhD Student at McGill and Mila with a concentration on *generative AI*, *graph neural networks*, and applications to *physics*, *materials science*, and *chemistry*. Focused on theory-informed development of ML models and their practical implementations, informed by a diverse background in physics research and software engineering.

Education

McGill University / Mila – Quebec AI Institute *Montreal, QC*

Supervisor: Siamak Ravanbakhsh

Ph.D. Computer Science, *CGPA: 4.0* *Sep 2022 - Present*

- Developing new geometric graph neural networks and applying them to physics and chemistry problems. Applying generative AI to drug discovery and discovering new crystalline materials.

M.Sc. Computer Science, *CGPA: 4.0* *Sep 2020 – Aug 2022*

- Thesis: Symmetries in graph neural networks and deep learning for heterogeneous network data.

University of British Columbia *Vancouver, BC*

B.Sc. Combined Honours in Computer Science and Physics, *CGPA: 92%* *Sep 2014 - May 2019*

- Thesis: likelihood approach to subatomic particle identification using Cherenkov detector simulations.

Publications

Major Conferences

- Energy loss functions for physical systems
  *SO Kaba, K Sareen, **D Levy**, S Ravanbakhsh.* NeurIPS 2025.
- SymmCD: Symmetry-Preserving Crystal Generation with Diffusion Models
  ***D Levy**, SS Panigrahi, SO Oumar Kaba, Q Zhu, M Galkin, S Miret, S Ravanbakhsh.* ICLR 2025.
- E (3)-Equivariant Mesh Neural Networks
  *T Trang, NK Ngo, **D Levy**, TN Vo, S Ravanbakhsh, TS Hy.* AIStats 2024.

Peer-reviewed Workshops

- LeMat-GenBench: Bridging the gap between crystal generation and materials discovery
  *A Duval, S Betala, SP Gleason, A Xu, G. Channing, **D Levy**, A Ramlaoui, C Fourrier, CK Joshi, N Kazeev, SO Kaba, F Therrien, A Hernández-García, R Mercado, NMA Krishnan*
  AI for Accelerated Materials Design – NeurIPS 2025
- Symmetry-Aware Generative Modeling through Learned Canonicalization.
  *K Sareen, **D Levy**, AK Mondal, SO Kaba, T Akhound-Sadegh, S Ravanbakhsh*
  Symmetry and Geometry in Neural Representations – NeurIPS 2024
- Using Multiple Vector Channels Improves E (n)-Equivariant Graph Neural Networks.
  ***D Levy**, SO Kaba, C Gonzales, S Miret, S Ravanbakhsh* Machine Learning for Astrophysics – ICML 2023
- Molecular fragment-based diffusion model for drug discovery
  ***D Levy**, J Rector-Brooks.* Machine Learning for Drug Discovery workshop – ICLR 2023

Journal Articles

- Single neutron transfer on 23Ne and its relevance for the pathway of nucleosynthesis in astrophysical X-ray bursts.
  G Lotay, et al., 2022., Physics Letters B 833, 137361

Research and Work Experience

Amazon *Vancouver, BC*

Software Development Engineer *Sep 2019 – Aug 2020*

- Developed and maintained highly critical tax-related services used across Amazon.
- Took ownership across all elements of software lifecycle, with an emphasis on continuous deployment and high performance, scalability, and availability.

University of Toronto Department of Physics, ATLAS group *Toronto, ON*

NSERC USRA Research Intern, Supervised by Pekka Sinervo *May – Aug 2019*

- Investigated a novel approach to Higgs boson tagging as part of an LHC search for exotic particles.

Thoughtexchange Vancouver, BC

Software Developer Intern *May - Aug 2018*

- Full stack development of new features to Thoughtexchange app. Implemented an NLP algorithm to sort users and created APIs to help handle moderation and phone number authentication.

Analysis and Prototyping Software Engineer Intern *Sep - Dec 2017*

- Developed ML-based methods to discover and classify common use patterns for the Thoughtexchange app. Designed interactive visualizations of results, used to direct app development

TRIUMF *Vancouver, BC*

Research Intern, Supervised by Adam Garnsworthy *Jan – Aug 2017*

- Analysed gamma-ray spectra to evaluate nuclear structure in a Coulomb excitation experiment. Calibrated detectors. Supervised experimental shifts.

Selected Awards and Achievements

- FRQNT Doctoral Training Scholarship ($25,000/year, 4 years) *2023 – 2027*
- NSERC Canada Graduate Scholarship – Master's program ($17,500) *2021-2022*
- NSERC Undergraduate Student Research Award ($6000) *2019*
- UBC Trek Excellence Scholarship for Continuing Students *(top 5% of faculty)* *2015, 2016, 2018*
- UBC Dean's Honour List *2014 – 2018*
- Dorothy Gladys Studer Memorial Scholarship *(Highest standing among 3rd year physics)* *2018*

Activities

- TA for UBC undergraduate course *CPSC 121: Models of computation* (2016)
- Presented talk at *Cosmic Connections: a ML X Astrophysics Symposium at the Simons Foundation* (2023)
- Reviewer for workshops: *ICLR 2022 Blog Track*, *Workshop on Machine Learning for Astrophysics – ICML 2023*, *Workshop on AI for Accelerated Materials Design – NeurIPS 2023* and *NeurIPS 2025*, *Frontiers in Probabilistic Inference Workshop – NeurIPS 2025* and *ICLR 2025*

Skills

- Machine Learning: experience with graph neural networks, generative modelling, 3D equivariant GNNs, diffusion models, flow matching models.
- Research in materials discovery, crystallography, drug discovery, and physics simulations
- Python, PyTorch, Java, Javascript, C++, Pandas, NumPy