

Gary Tom

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I am a highly-motivated PhD student with a passion for applying evidence-based strategies to solve impactful problems. With a strong background in chemistry, physics, and machine learning, I am well-equipped to tackle challenging scientific problems with AI based approaches. My current interests are in the field of drug/materials design, as well as probabilistic and graph-based modelling of chemical properties. More broadly, I want to explore new fields in a dynamic research environment and have the chance to learn and try new things.

Relevant Experience

Aspuru-Guzik Matter Lab · University of Toronto

TORONTO, ON

PhD Graduate Researcher

May 2020 – present

- ◆ Creating a package for probabilistic prediction on small datasets of molecules using TensorFlow. Examining the calibration of uncertainty in the models and their effects on Bayesian optimization and generalizability [1, 2].
- ◆ Implementing string-based generative models in PyTorch for realistic materials design tasks, ie. drug design, OLED and solar cell molecule design [3].
- ◆ Developing generative models (genetic algorithms and VAE) for low-data inverse design of molecules.
- ◆ Studying multi-objective optimization of chemical properties using various scalarizing functions. Accepted as poster for NeurIPS workshop [5].
- ◆ Engineering molecular graph features based on electronic structures with the goal of improving performance of graph-based neural networks on chemical structures.

SandboxAQ

TORONTO (REMOTE), ON

AI PhD Resident

May – Aug 2023

- ◆ Developed an equivariant 3D graph neural network for predicting the binding affinity of potential drug candidates to target proteins binding pockets, as part of research project with AQBioSim team.
- ◆ Collaborated with computational team to perform active learning virtual screens on large libraries of organic compounds. Delivered major milestone for client, with top suggestions for possible new pharmaceuticals.
- ◆ Methods developed are patent pending, with a manuscript currently under peer-review [4].

Laboratory for Atomic Imaging Research · University of British Columbia

VANCOUVER, BC

MSc Graduate Researcher

Aug 2017 – Apr 2020

- ◆ Studied the luminescence of single organic photovoltaic molecules using scanning tunneling microscopy (STM). Presented findings as an invited speaker at IVC 2019 [7].
- ◆ Developed MATLAB analysis script to study strain in graphene samples, characterized by STM [8].

Laboratory for Atomic Imaging Research · University of British Columbia

VANCOUVER, BC

Natural Science and Engineering Research Council (NSERC) Summer Researcher

May – Aug 2016

- ◆ Implemented deconvolution algorithms to analyze scanning tunneling spectroscopy data of organic semiconductors. Algorithms reduced data processing time and improved overall accuracy of results [10].

Hendricks Lab · McGill University

MONTREAL, QC

Undergraduate Research Student

Sep 2015 – Apr 2016

- ◆ Created a robotics control system for fluorescence microscope and laser tweezers used for studying protein mechanics in biological samples.

Institute for Research on Exoplanets · Université de Montréal

MONTREAL, QC

Trottier Summer Intern

May – Aug 2015

- ◆ Created a suite of IDL scripts that analyzed large data sets of astronomical surveys to identify young star candidates based on X-ray and UV luminosities.
- ◆ Used Bayesian analysis of stellar velocities and positions to identify associations of co-moving stars.
- ◆ Identified over 300 previously unreported young star candidate targets for exoplanet imaging.

Technical Skills

- ◆ Proficient in Python, MATLAB, IDL, and LabView. Experience with FORTRAN, Java, and C.
 - ◆ Highly experienced with common ML frameworks in Python: TensorFlow/Keras, PyTorch, JAX/FLAX, and scikit-learn.
 - ◆ Experience with probabilistic prediction and classification models such as GPyTorch, and TensorFlow-Probability.
 - ◆ Experience with generative modelling: variational autoencoder, genetic algorithms, and reinforcement learning. Worked with language models and graph-based models (PyTorch-Geometric) applied to chemical information.
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Education

University of Toronto	TORONTO, ON
PhD in Physical Chemistry (Supervisor: Prof Alán Aspuru-Guzik)	2020 – present
Studying the application of machine learning algorithms in accelerating drug and materials discovery.	
University of British Columbia	VANCOUVER, BC
MSc in Physics (Supervisor: Prof Sarah Burke)	2017 – 2020
Thesis: <i>Scanning probe microscopy study of organic semiconducting molecules.</i>	
McGill University	MONTRÉAL, QC
BSc Honours in Physics (Supervisor: Prof Peter Grütter)	2013 – 2017
Graduated with First Class Honours, along with a minor in Interdisciplinary Life Sciences.	

Select Honours and Awards

Postgraduate Scholarship Doctoral (PGS-D)	2021–present
Awarded by NSERC, provides 3 years of financial support for doctoral research in natural sciences and engineering.	
Vector Research Grant	2023
Awarded by the Vector Institute, provides financial support to researchers involved in applied AI research.	
Ontario Graduate Scholarship	2020
Awarded by the Province of Ontario and the University of Toronto, for academic excellence in graduate studies.	
Alexander Graham Bell Canada Graduate Scholarship–Master’s (CGS-M)	2018–2019
Awarded by NSERC, for academic and research excellence in graduate studies.	
Quantum Electronics and Technology Student Initiative	2017–2020
Awarded by the Stewart Blusson Quantum Matter Institute (SBQMI), a major 3-year scholarship for graduate studies in quantum materials at UBC.	
Undergraduate Summer Research Award	2016
Awarded by NSERC, and Fonds de recherche du Québec-Nature et technologies, to nurture and develop research potential undergraduates by funding summer research positions.	
Trottier Excellence Grant	2015
Awarded by Trottier Family Foundation to fund a summer internship at the Institute for Research on Exoplanets.	

Select Publications and Talks

1. **G. Tom**, R. J. Hickman, A. Zinzuwadia, A. Mohajeri, B. Sanchez-Lengeling, and A. Aspuru-Guzik. Calibration and generalizability of probabilistic models on low-data chemical datasets with DIONYSUS. *Digital Discovery*, 2:759–774, 2023.
2. R.-R. Griffiths, L. Klarner, H. B. Moss, A. Ravuri, S. Truong, S. Stanton, **G. Tom**, et al. GAUCHE: A library for gaussian processes in chemistry. *Advances in Neural Information Processing Systems (NeurIPS)*, 2023.
3. A. Nigam, R. Pollice, **G. Tom**, K. Jorner, J. Willes, L. A. Thiede, A. Kundaje, and A. Aspuru-Guzik. Tartarus: A benchmarking platform for realistic and practical inverse molecular design. *Advances in Neural Information Processing Systems (NeurIPS)*, 2023.
4. J. E. Crivelli-Decker, Z. Beckwith, **G. Tom**, L. Le, S. Khuttan, R. Salomon-Ferrer, J. Beall, R. Gómez-Bombarelli, and A. Bortolato. Machine learning guided AQFEP: A fast efficient absolute free energy perturbation solution for virtual screening. *Manuscript under review for publication*, 2023.
5. N. Kusanda, **G. Tom**, R. J. Hickman, A. Nigam, K. Jorner, and A. Aspuru-Guzik. Assessing multi-objective optimization of molecules with genetic algorithms against relevant baselines. *Advances in Neural Information Processing Systems (NeurIPS)*, AI4Materials Workshop, 2022.
6. M. DeJong, A. Price, E. Mårsell, **G. Tom**, G. Nguyen, E. Johnson, and S. Burke. Small molecule binding to surface-supported single-site transition-metal reaction centres. *Nature Communications*, 13(1):1–10, 2022.
7. **G. Tom**, E. Mårsell, G. D. Nguyen, T. Roussy, K. A. Cochrane, and S. A. Burke. Tunneling-induced luminescence on photovoltaic molecular heterodimers. 21st International Vacuum Conference (invited talk), 2019.
8. P. Nigge, A. Qu, É. Lantagne-Hurtubise, E. Mårsell, S. Link, **G. Tom**, M. Zonno, M. Michiardi, M. Schneider, S. Zhdanovich, U. Starke, C. Gutiérrez, D. Bonn, S. A. Burke, M. Franz, and A. Damascelli. Room temperature strain-induced Landau levels in graphene on a wafer-scale platform. *Science Advances*, 5(11):eaaw5593, 2019.