

Kyle Mills

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kyle@kylemills.net

github.com/millskyle

languages

Python, SQL, C,
C++, Fortran, BASH,
PHP, JavaScript
(with AngularJS),
HTML

skills/ software/tools

TensorFlow,
PyTorch, Git,
Jupyter, MPI,
OpenMP, CUDA,
Python (Numpy,
Matplotlib, etc.),
Linux, Matlab,
Gnuplot, \LaTeX ,
Slack, Blender, web
design,
programming,
scripting, teaching,
graphic design

References
available upon
request

education

- 2015–
2021 **Ph.D.** Modelling and Computational Science *Ontario Tech University*
Transferred from M.Sc. to Ph.D. in March 2017.
- Visiting scholar at the National Research Council Canada.
- Reinforcement Learning Researcher at 1QBit, Vancouver, British Columbia
- Postgraduate Affiliate with Vector Institute for Artificial Intelligence, Toronto, Ontario
- 2011–
2015 **B.Sc.** Physics (Honours) *University of Ontario Institute of Technology*
Minor in Mathematics
Graduated with **Highest Distinction** with 3.92 GPA.
President's list 2011, 2013, 2014, and 2015.

publications

- 2020 **Adversarial generation of mesoscale surfaces from small scale chemical motifs**
Kyle Mills, Corneel Casert, Isaac Tamblyn
J. Phys. Chem. C, 124, 42, 23158–23163. Machine Learning In Physical Chemistry Special Issue
- 2020 **Finding the ground state of spin Hamiltonians with reinforcement learning**
Kyle Mills, Pooya Ronagh, Isaac Tamblyn
Nature Machine Intelligence, 2, 509-517(2020). Sept. 2020 cover article.
- 2020 **Crystal Site Feature Embedding Enables Deep Image Recognition Based Exploration of Chemical Spaces Exceeding One Billion Compounds**
Mikhail Askerka, Kevin Ryczko, Oleksandr Voznyy, Kyle Mills, Isaac Tamblyn, and Edward H. Sargent
Matter 3, 2, 433-448
- 2019 **Extensive deep neural networks for transferring small scale learning to large scale systems**
Kyle Mills, Kevin Ryczko, Iryna Luchak, Adam Domurad, Chris Beeler, and Isaac Tamblyn
Chem. Sci., 2019, 10, 4129-4140. Edge (cover) article
- 2018 **Deep neural networks for direct, featureless learning through observation: the case of 2d spin models**
Kyle Mills and Isaac Tamblyn
Phys. Rev. E 97, 032119.
- 2018 **Convolutional neural networks for atomistic systems**
Kevin Ryczko, Kyle Mills, Iryna Luchak, Christa Homenick, and Isaac Tamblyn
Comp. Mat. Sci. 149, 134-142.
- 2017 **Deep learning and the Schrödinger equation**
Kyle Mills, Michael Spanner, and Isaac Tamblyn
Phys. Rev. A 96, 042113. Editor's Suggestion.

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publications, continued

- 2021 **Optimizing thermodynamic trajectories using evolutionary reinforcement learning**
Chris Beeler, Uladzimir Yahorau, Rory Coles, Kyle Mills, Stephen Whitelam, Isaac Tamblyn
arXiv: 1903.08543
- 2020 **Optical lattice experiments at unobserved conditions and scales through generative adversarial deep learning**
Corneel Casert, Kyle Mills, Tom Vieijra, Jan Ryckebusch, Isaac Tamblyn
arXiv: 2002.07055
- 2021 **Weakly-supervised multi-class object localization using only object counts as labels**
Corneel Casert, Kyle Mills, Tom Vieijra, Jan Ryckebusch, Isaac Tamblyn
arXiv: 2102.11743
- 2017 **Phase space sampling and operator confidence with generative adversarial networks**
Kyle Mills and Isaac Tamblyn
arXiv: 1710.08053

presentations

- 2019 **Adversarial generation of mesoscale surfaces from small scale chemical motifs**
NeurIPS 2019 Machine Learning for Physical Sciences Workshop, Vancouver.
- 2018 **Extensive deep neural networks**
Computational Materials North, Montréal, Quebec, Canada
- 2017 **Learning the Schrödinger equation with deep neural networks**
Canadian Chemistry Conference, Toronto, Ontario, Canada
Presented research at Canadian Society for Chemistry's annual conference.
- 2017 **Deep learning and the Schrödinger equation**
American Physical Society March Meeting, New Orleans, Louisiana, USA
Presented research at International APS March Meeting.
- 2015 **Designing lightweight aluminum composites: A first principles density functional theory approach.**
Conference of Metallurgists, Toronto, Ontario, Canada
Presented research at Canadian metallurgy conference in the computational materials science symposium.
- 2015 **Comparison of theoretical methods with boron nitride nanostructures.**
Undergraduate Summer Research Showcase, Oshawa, Ontario, Canada
Competitive poster presentation at the University of Ontario Institute of Technology
- 2015 **Long-lived ligand-to metal charge-transfer state of an oxidovanadate complex**
Designed cover image chosen to appear on the cover of the July 30, 2015 issue of the Journal of Physical Chemistry C.
- 2014 **Aluminum wetting of hexagonal boron nitride.**
National Research Council Security and Disruptive Technologies 2014 Tech Day, Ottawa, Ontario
First place winning poster in competitive poster presentation.
- 2014 **Designing lightweight aluminum composites: A density functional theory approach.**
Canadian Undergraduate Physics Conference, Queen's University, Kingston, Ontario
Presented original research in a competitive talk aimed at other Canadian undergraduate physics students.
- 2014 **Aluminum wetting of hexagonal boron nitride.**
Undergraduate Summer Research Showcase, Oshawa, Ontario
Competitive poster presentation at the University of Ontario Institute of Technology.

experience

- 2019–
present **Postgraduate Affiliate** *Vector Institute, Toronto, Ontario, Canada*
- Conduct research in affiliation with Vector Institute for Artificial Intelligence
- 2018–
present **Researcher, Applied Maths and Reinforcement Learning** *1QBit, Vancouver, British Columbia, Canada*
- Mitacs intern
- Develop and implement reinforcement learning (RL) algorithms
- Develop and implement RL and energy-based models on quantum computer hardware
- 2016–
present **Visiting scholar** *National Research Council Canada, Ottawa, Ontario*
- Conduct research and collaborate with researchers at the National Research Council Canada.
- 2013–
2017 **Teaching assistant** *UOIT*
- Supervise laboratory experiments for physics courses.
- Design and instruct introductory Raspberry Pi physics laboratory experiments.
- Conduct tutorials to assist students in understanding advanced physics concepts.
- 2015–
2016 **Programming/Electronics course content design** *UOIT*
- Design course content to introduce Faculty of Education students to programming and electronics.
- Lead tutorials and extra-curricular workshops to teach students about Linux and Raspberry Pis.
- 2014 **Research assistant** *Computational Laboratory for Energy and Nanoscience*
- Performed large-scale, distributed computations of atomic-scale materials science problems, working toward the design of lightweight aluminum composites.
- Worked in collaboration with researchers at National Research Council, Ottawa, Ontario.
- Experience building and running highly parallelized programs.
- 2012–
2014 **Summer student, Energy Settlements Dept.** *Veridian Connections, Ajax, ON*
- SQL database administration for reports, audits, automation, etc.
- Assisted system administrator with server maintenance.
- Wrote scripts to automate tasks and increase employee efficiency.
- Assisted with generation, validation, and distribution of electricity bills.

awards

- 2019–21 **NSERC Alexander Graham Bell Canada Graduate Scholarship Doctoral (CGS-D)**
National scholarship awarded to students based on academic performance and research potential.
- 2019–20 **Vector Institute for Artificial Intelligence Postgraduate Affiliate Award**
Affiliate program for postgraduate students conducting research in the field of artificial intelligence.
- 2019 **Ontario Graduate Scholarship**
Provincial scholarship awarded to students based on academic performance and research potential.
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- 2016 **Ontario Graduate Scholarship**
Provincial scholarship awarded to students based on academic performance and research potential.
- 2016 **NSERC Alexander Graham Bell Canada Graduate Scholarship Master's (CGS-M)**
National scholarship awarded to 2 top performing graduate students.
- 2015 **Ontario Graduate Scholarship**
Provincial scholarship awarded to students based on academic performance and research potential.
- 2014 **Rotoract UOIT Scholarship**
Scholarship awarded to the 16 top-performing students at the University of Ontario Institute of Technology.
- 2014 **NSERC-CSRNG Undergraduate Student Research Award (USRA)**
National award given to students who show research potential and excellent academic performance
- 2011 **UOIT Entrance Scholarship**
Awarded to students with a greater than 90% high school average upon entrance

notable projects and extra-curricular

- 2016 **Vice President, UOIT Graduate Student Council**
- Assisted in organization of graduate student research conference
 - Represent graduate student body in meetings with administration
- 2015 **Interval Scheduling Algorithm with Applied Constraints**
- Lead a team in developing a scheduling web app that utilizes Monte Carlo methods and graph theory to optimize students' schedules.
- 2015 **Science Rendezvous Weather Balloon Launch (HABEX) Team Lead**
- Coordinated and lead the launch team of a HABEX weather balloon for UOIT's Science Rendezvous.
 - Coordinated with local authorities to ensure a safe launch.
 - Represented UOIT Physics to community members and families.
 - Designed website displaying results and footage from the activity (<http://uoitphysics.ca/balloon>).
 - Perform interviews with local media contacts.
- 2015–
2016 **President (Founding), Academic Skills Club**
- Design and teach workshops for undergraduate and graduate students to develop useful scientific research and programming skills.
- 2014–
2015 **Vice President, UOIT Physics Society**
- Build and maintain website (uoitphysics.ca), manage social networking.
 - Build email distribution system for mailing list (PHP, MySQL, HTML)
 - Act effectively as main contact between physics faculty and students.