Riley Hickman

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EDUCATION

University of Toronto **Toronto, Ontario, Canada**
Ph.D. student in Physical Chemistry *Sept 2018 - Present*

CGPA: 4.0/4.0
Advisor: Prof. Alán Aspuru-Guzik

Carleton University **Ottawa, Ontario, Canada**
B.Sc. Honours in Chemistry with minor in Physics *Sept 2014 - Apr 2018*

CGPA: 3.9/4.0 (Senate Medal - Undergraduate)
Honours project: General formalism for vibronic Hamiltonians in tetragonal symmetry and beyond
Advisor: Prof. Tao Zeng

RESEARCH EXPERIENCE

Graduate Researcher *Advisor: Prof. Alán Aspuru-Guzik*

- Enhancing the efficiency of self-driving laboratories by devising machine learning algorithms that make use of heterogeneous data
- Interleaving machine learning with affordable quantum chemistry methods to enable efficient virtual screening of organic electronic candidate molecules
- Theoretical studies of chemical media for a novel annealing droplet computer based on the Ising model

Undergraduate Researcher *Advisor: Prof. Tao Zeng*

- Deriving arbitrarily-high-order expansion formulas in vibrational coordinates for the Jahn-Teller and pseudo-Jahn-Teller vibronic Hamiltonians of polyatomic systems
- Symbolic programming in Python for automatic generation of vibronic Hamiltonians

Undergraduate Researcher *Advisor: Prof. Séan Barry*

- Assisting Ph.D. students in research involving chemical vapour deposition (CVD) and atomic layer deposition (ALD)
- Preparation of CVD/ALD precursor molecules using various synthetic techniques
- Characterization and volatility testing using mass spectrometry, NMR, thermogravametric analysis, and differential scanning calorimetry

PREPRINTS AND MANUSCRIPTS IN PREPARATION

3. F. Häse, M. Aldeghi, **R. J. Hickman**, L. M. Roch, M. Christensen, E. Liles, J. E. Hein, A. Aspuru-Guzik, “Olympus: benchmarking optimization algorithms for autonomous experimentation", *In preparation*.

2. **R. J. Hickman**, F. Häse, L. M. Roch, A. Aspuru-Guzik, “Gemini: Dynamic bias correction for autonomous experimentation", *In preparation*.

1. S. Y. Guo, P. Friederich, Y. Cao, T. Wu, C. Forman, D. Mendoza, M. Degroote, A. Cavell, V. Krasecki,

R. J. Hickman, A. Sharma, L. Cronin, N. Gianneschi, R. Goldsmith, A. Aspuru-Guzik, "A molecular computing approach to solving optimization problems via programmable microdroplet arrays", *ChemRxiv. Preprint.* **2019**, https://doi.org/10.264334/chemrxiv.10250897.v1

PEER-REVIEWED PUBLICATIONS

4. A. C. Cavell, V. K. Krasecki, G. Li, A. Sharma, H. Sun, M. P. Thompson, C. J. Forman, H. Sun, S. Y. Guo, **R. J. Hickman**, K. A. Parrish, A. Aspuru-Guzik, L. Cronin, N. C. Gianneschi, R. H. Goldsmith, "Optical monitoring of polymerizations in droplets with high dynamic range", *Chem. Sci.* **2020**, *11*, 2647-2656.

3. R. A. Lang, **R. J. Hickman**, T. Zeng, "VHEGEN: A vibronic Hamiltonian expansion generator for trigonal and tetragonal polyatomic systems", *Comput. Phys. Commun.* **2019**, *247*, 106946.

2. **R. J. Hickman**, R. A. Lang, T. Zeng, "General formalism for vibronic Hamiltonians in tetragonal symmetry and beyond", *Phys. Chem. Chem. Phys*. **2018**, *20*, 12312-12322.

1. T. Zeng, **R. J. Hickman**, A. Kadri, I, Seidu, "General formalism of vibronic Hamiltonians for tetrahedral and octahedral systems: problems that involve *T*, *E* states and *t*, *e* vibrations", *J. Chem. Theory Comput.* **2017**, *13*, 5004-5018.

ORAL AND POSTER PRESENTATIONS

3. F. Häse, **R. J. Hickman**, M. Aldeghi*, E. Liles, L. M. Roch, J. E. Hein, A. Aspuru-Guzik. Olympus: A toolkit for benchmarking optimization algorithms on experimentally derived surfaces. AI Powered Drug Discovery and Manufacturing, Cambridge, M.A., February 2020. (Poster)

2. **R. J. Hickman***, J. Proppe, C. J. Stein, T. Gaudin, M. Head-Gordon, A. Aspuru-Guzik. Machine learning range-separated hybrid functionals for high-throughput calculations. 9th Molecular Quantum Mechanics Conference, Heidelberg, Germany, July 2019. (Poster)

1. J. Proppe*, C. J. Stein, T. Gaudin, **R. J. Hickman**, M. Head-Gordon, A. Aspuru-Guzik. Automated generation of benchmark sets guided by a Bayesian decision maker. 9th Molecular Quantum Mechanics Conference, Heidelberg, Germany, July 2019. (Poster)

* Presenter

AWARDS AND SCHOLARSHIPS

- 2019 School of Graduate Studies Conference Grant ($1150)
- 2019-2022 NSERC Postgraduate Scholarship - Doctoral (PGS-D) ($63000)
- 2018-2019 NSERC Alexander Graham Bell Canada Graduate Scholarship - Masters (CGS-M) ($17500)
- 2018 University of Toronto Chemistry Departmental Award ($2000)
- 2018 Society of Chemical Industry Award
- 2017 Canadian Society for Chemistry Medal
- 2017 Janet M. Holmes Memorial Scholarship ($1000)
- 2016 Dr. M. Ralph Berke Award ($250)

TEACHING EXPERIENCE

Tutorial Teaching Assistant — **Toronto, Ontario, Canada**
University of Toronto, Department of Computer Science — *Sept 2019 - Present*

- Computing for Science (CSC198)
- Taught undergraduate students scientific programming in Python
- Design and assembly of titration robot controlled by computer vision software

Tutorial Teaching Assistant **Toronto, Ontario, Canada**
University of Toronto, Department of Chemistry *Jan 2019 - Apr 2019*

- 2nd year Quantum Mechanics (CHM223)
- Led problem set review style tutorial sessions for a section of 20 students

Laboratory Teaching Assistant **Ottawa, Ontario, Canada**
Carleton University, Department of Chemistry *Sept 2017 - Apr 2018*

- 2nd year Organic Chemistry Laboratory (CHM 2223/2224)
- Preparation and presentastion of pre-lab lecture and quiz material, grading lab reports
- Monitoring and assisting students during experiments

KEY SKILLS

Programming Language	Python, C++, Bash
Machine Learning Libraries	TensorFlow, Keras, PyTorch
Chemistry Software	QChem, ORCA, GAMESS, RDKit, Open Babel
Web Based Language	HTML, CSS, PHP

VOLUNTARY ACTIVITIES

Career Mentor **Ottawa, Ontario, Canada**
Science Student Success Centre, Carleton University *Sept 2017 - Apr 2018*

- Working with students on an individual basis or in small groups to help them define and achieve their academic, career, and social goals
- Preparation and presentation of skill building workshops (Topics: LaTeX, MATLAB)

Emergency Department Volunteer **Ottawa, Ontario, Canada**
Queensway Carleton Hospital *Nov 2016 - Sept 2018*

- Preparing paperwork for physicians and other healthcare professionals
- Patient escorts, visitor escorts, patient lookup, patient meal preparation