Alexander Ibrahim

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Education

PhD, Physics, **University of Waterloo**, *Waterloo, ON, Canada* *Sep 2018 – Sep 2024*
Thesis topic: Creating machine-learned potentials for high-performance simulations of solid parahydrogen

BSc, Physics, **McMaster University**, *Hamilton, ON, Canada* *Sep 2013 – May 2018*

Experience

Postdoctoral Research Scientist *Waterloo, ON, Canada*
University of Waterloo *Sep 2024 – Jun 2025*

- Used C++20 and CMake to write a 30k LOC quantum circuit simulator from scratch, which was put on GitHub, unit tested with Catch2, compiled on Linux using GCC and Clang, and checked using Asan and Msan
- Developed CI pipeline with GitHub Actions and Docker, with automated formatting, building, and unit testing
- Used NumPy, SciPy, Matplotlib, and pytest to analyze results and perform visualization
- Used Slurm to run jobs for QPE and VQE simulations on HPC ComputeCanada supercomputer clusters
- Collaborated with and was advised by researchers at qBraid to plan research direction, resulting in a paper
- Used OpenFermion, Tangelo, and Qiskit to map Hamiltonians of dipolar coplanar rotors to qubits and create Trotterized time evolution operators

Graduate Research Scientist *Waterloo, ON, Canada*
University of Waterloo *Jun 2018 – Sep 2024*

- Used NumPy, SciPy, Matplotlib, pytest, and SQL to perform data analysis, error analysis, and visualization
- Trained neural network many-body potentials from scratch using Python and PyTorch in virtual environments, which were ported to C++ LibTorch for simulations, and made available on GitHub
- Wrote a C++20 header-only templated Path Integral Monte Carlo simulation project, which was put on GitHub and packaged with CMake, using Catch2 for unit testing
- Used Slurm to perform simulations on thousands of cores on HPC ComputeCanada supercomputing clusters
- Performed quantum chemistry CCSD(T) calculations on HPC supercomputing clusters to find non-additive many-body interaction energies for parahydrogen molecules, creating a new dataset available on Zenodo
- Used domain knowledge of physics to choose data that improves model quality using fewer samples, and create transformation layers that improve predictions for testing data spanning several orders of magnitude

Co-op Research Scientist *Maple Ridge, BC, Canada*
E-One Moli Energy Canada Ltd *Jan 2016 – Aug 2016*

- Gave bimonthly presentations explaining battery research to non-technical staff, executives, and scientists
- Used Python and SciPy to analyze physical and chemical properties of lithium-ion batteries

Other Experience

Co-op Research Scientist *Hamilton, ON, Canada*
McMaster University *Sep 2017 – Dec 2017*

- Used Python to create novel methods to analytically solve the infinitely periodic Schrödinger Equation

Co-op Research Scientist *Edmonton, AB, Canada*
University of Alberta *May 2016 – Aug 2016*

- Used the pseudopotential method to improve the convergence rates of wave function calculations

Co-op Research Scientist *Hamilton, ON, Canada*
McMaster University *May 2015 – Aug 2015*

- Grew crystals with a floating-zone furnace, and measured their magnetic and crystallographic properties

Selected Publications

M. S. Moeed and J. Brown and **A. Ibrahim** and E. V. B. D. Oliveira and P.-N. Roy, "Qubit encodings for lattices of dipolar planar rotors," [submitted to *J. Chem. Phys.* arxiv]

A. Ibrahim and P.-N. Roy, "Path-integral Monte Carlo simulations of solid parahydrogen using two-body, three-body, and four-body *ab initio* interaction potential energy surfaces," *J. Chem. Phys.* **162**, 164503, (2025). [arxiv]

A. Ibrahim and P.-N. Roy, "A neural network-based four-body potential energy surface for parahydrogen," *J. Chem. Phys.* **160**, 244308, (2024). [arxiv]

A. Ibrahim and P.-N. Roy, "Equation of state of solid parahydrogen using *ab initio* two-body and three-body interaction potentials," *J. Chem. Phys.* **157**, 174503, (2022). [arxiv]

A. Ibrahim and P.-N. Roy, "Three-body potential energy surface for *para*-hydrogen," *J. Chem. Phys.* **156**, 044301, (2022). [arxiv]

A. Ibrahim and F. Marsiglio, "A quantum moat barrier, realized with a finite square well," *Can. J. Phys.* **99**, 1035-1041, (2021). [arxiv]

A. Ibrahim and L. Wang and T. Halverson and R. J. Le Roy and P.-N. Roy, "Equation of state and first principles prediction of the vibrational matrix shift of solid parahydrogen," *J. Chem. Phys.* **151**, 244501, (2019). [arxiv]

A. Ibrahim and D. W. L. Sprung and G. V. Morozov, "Construction and Floquet-Bloch analysis of analytically solvable Hill equations with smooth potentials, *J. Opt. Soc. Am. B*, **35**, 1223-1232, (2018).

A. Ibrahim and F. Marsiglio, "Double well potentials with a quantum moat barrier or a quantum wall barrier give rise to similar entangled wave functions," *Am. J. Phys.*, **86**, 180-185, (2018). [arxiv]

Conferences

A. Ibrahim and P.-N. Roy, "Path-integral Monte Carlo simulations of solid parahydrogen using many-body interaction potentials." 38^{th} Annual Symposium on Chemical Physics. University of Waterloo, Waterloo ON, Canada. Poster (Nov 2024).

A. Ibrahim and P.-N. Roy, "Many-body potential energy surfaces for parahydrogen, and simulations of solid parahydrogen." 30^{th} Canadian Symposium on Theoretical and Computational Chemistry. Dalhousie University, Halifax NS, Canada. Poster. (Jul 2024).

A. Ibrahim and P.-N. Roy, "Creating a neural network-based four-body *ab initio* potential energy surface for parahydrogen." 37^{th} Annual Symposium on Chemical Physics. University of Waterloo, Waterloo ON, Canada. Poster (Nov 2023).

A. Ibrahim and P.-N. Roy, "The effects of three-body interactions in simulations of solid parahydrogen." 12^{th} Triennial Congress of the World Association of Theoretical and Computational Chemists. Vancouver Convention Centre, Vancouver BC, Canada. Poster (Jul 2022).

A. Ibrahim and P.-N. Roy, "Calculating the equation of state of solid parahydrogen using *ab initio* many-body interaction potentials." 36^{th} Annual Symposium on Chemical Physics. University of Waterloo, Waterloo ON, Canada. Poster (Nov 2022).

A. Ibrahim and P.-N. Roy, "Equation of state and vibrational matrix shift of solid parahydrogen." 35^{th} Annual Symposium on Chemical Physics. University of Waterloo, Waterloo ON, Canada. Poster (Nov 2019).

A. Ibrahim and P.-N. Roy, "Equation of state and first principles prediction of the vibrational matrix shift of solid parahydrogen." 45^{th} International Congress of Theoretical Chemists of Latin Expression. Concordia University, Montreal QC, Canada. Poster (Aug 2019).

A. Ibrahim and F. Marsiglio, "Particles bumping into moats: Similarity of wave function solutions of positive and negative barriers." Undergraduate Summer Student Poster Display. University of Alberta, Edmonton AB, Canada. Poster (Aug 2017).

A. Ibrahim and G. Luke, "Crystal growth of spin ice pyrochlores using a floating-zone furnace." 56^{th} Annual Canadian Undergraduate Physics Conference. Trent University, Peterborough ON, Canada. Poster (Oct 2015).

Projects

kettle *github.com/AlexanderIbrahim1/kettle*

- Quantum circuit simulator written in C++20
- Packaged using CMake, extensively unit tested using Catch2, with documentation and examples
- Uses CI pipeline with GitHub Actions and Docker, with automated formatting, building, and unit testing
- Features include creating quantum circuits using standard gates, manipulating quantum circuits, simulating statevectors and density matrices, performing measurements, allowing classical control flow, and applying variational algorithms
- Used to perform QPE and VQE simulations, resulting in a publication

nn_fourbody_potential *github.com/AlexanderIbrahim1/nn_fourbody_potential*

- Neural network potential energy surface for four parahydrogen molecules, written with PyTorch
- Has training data available both in the GitHub repository and on Zenodo, with clear instructions and tooling to make it easy for other researchers to train the model from scratch
- Uses modern tools such as black, flake8 and pyright to maintain codebase quality
- Used in Path Integral Monte Carlo simulations of solid parahydrogen to get excellent agreement with experimental results

pimc-sim *github.com/AlexanderIbrahim1/pimc-sim*

- C++20 header-only template-heavy codebase for Path Integral Monte Carlo simulations of quantum solids
- Uses a C++ LibTorch implementation of the aforementioned many-body parahydrogen potential in PyTorch

monkey *github.com/AlexanderIbrahim1/monkey*

- A lexer, parser, interpreter, and compiler written from scratch in Python, following Thorsten Ball's books "Writing and Interpreter in Go" and "Writing a Compiler in Go"
- Uses unit testing in pytest and modern tools such as black, flake8 and pyright to maintain codebase quality

Technical Skills

Languages: Python, C++(11/14/17/20), Rust, Julia

Technologies: Linux, NumPy, SciPy, PyTorch, pytest, Qiskit, LibTorch, CMake, Catch2, Slurm, Bash, Git, GitHub Actions, CI/CD, Docker

Awards

Name	Source	Period Held	Value (CAD$)
GSPA Travel Award	University of Waterloo	05/2022	$ 500
NSERC CGSD	NSERC	05/2021 – 04/2024	$ 105000
President's Research Studentship	University of Waterloo	05/2021 – 04/2024	$ 15000
Graduate Research Studentship	University of Waterloo	05/2021 – 04/2024	$ 15000
Ontario Graduate Scholarship	Government of Ontario	09/2020 – 04/2021	$ 15000
Physics Department USRA	University of Alberta	05/2017 – 08/2017	$ 4500
NSERC IUSRA	NSERC	05/2016 – 08/2016	$ 4500
NSERC IUSRA	NSERC	01/2016 – 04/2016	$ 4500
NSERC USRA	NSERC	05/2015 – 08/2015	$ 4500
H. L. Hooker Scholarship	McMaster University	09/2015	$ 1500
A. B. McLay Scholarship	McMaster University	09/2015	$ 500