Alexander Ibrahim, Ph.D. | Canadian citizen

References available upon request

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Education

Sep 2018 – Sep 2024 ◇ **Ph.D., Physics**, University of Waterloo, *Waterloo, ON*
Thesis: *Path Integral Monte Carlo simulations of solid parahydrogen using many-body interaction potentials*
Supervisor: Dr. Pierre-Nicholas Roy
Grade: 95 %
- Performed quantum chemistry CCSD(T) calculations to find many-body interaction energies
- Used PyTorch and C++ LibTorch to create a neural network many-body potential for parahydrogen
- Wrote path-integral Monte Carlo simulation code in C++ to simulate solid parahydrogen
- Managed large-scale calculations on computing clusters using Slurm

Sep 2013 – May 2018 ◇ **Bachelor of Physics, Honours with Co-op**, McMaster University, *Hamilton, ON*

Employment History

Sep 2024 – Present ◇ **Postdoctoral Research Scientist**, University of Waterloo, *Waterloo, ON*
- Mapping systems of dipolar planar rotors to qubits, performing QPE and VQE simulations

Sep 2017 – Dec 2017 ◇ **Co-op Student Researcher**, McMaster University, *Hamilton, ON*
- Created novel methods to analytically solve the infinitely periodic Schrödinger Equation

May 2017 – Aug 2017 ◇ **Co-op Student Researcher**, University of Alberta, *Edmonton, AB*
- Used the pseudopotential method to improve the convergence rates of wave function calculations

Jan 2016 – Aug 2016 ◇ **Co-op Research Scientist**, E-One Moli Energy Canada Ltd, *Maple Ridge, BC*
- Studied the properties of a new binder material for silicon batteries, and analyzed their chemical properties
- Gave bimonthly presentations explaining results to other scientists and executives

May 2015 – Aug 2015 ◇ **Student Researcher**, McMaster University, *Hamilton, ON*
- Grew rare earth titanate single crystals with a floating-zone furnace
- Measured crystal magnetic properties using a superconducting quantum interference device (SQUID)

Skills

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

Tools ◇ Linux, NumPy, SciPy, PyTorch, pytest, Qiskit, LibTorch, CMake, Catch2, Slurm, Bash, Git, GitHub Actions, CI/CD

Selected Software Projects

- ◇ **kettle** : C++20 quantum circuit simulator, capable of QPE and variational simulations
- ◇ **nn_fourbody_potential** : neural network potential energy surface for four parahydrogen molecules
- ◇ **pimc-sim** : C++20 library for performing path-integral Monte Carlo simulations of quantum solids
- ◇ **elecstruct** : C++20 toy implementation of the Hartree-Fock algorithm

Journal Articles

1. **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).
2. **A. Ibrahim** and P.-N. Roy, "A neural network-based four-body potential energy surface for parahydrogen", *J. Chem. Phys.* **160**, 244308 (2024).
3. **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).
4. **A. Ibrahim** and P.-N. Roy, "Three-body potential energy surface for *para*-hydrogen", *J. Chem. Phys.* **156**, 044301 (2022).
5. **A. Ibrahim** and F. Marsiglio, "A quantum moat barrier, realized with a finite square well", *Can. J. Phys.* **99**, 1035–1041 (2021).
6. **A. Ibrahim**, L. Wang, T. Halverson, 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).
7. **A. Ibrahim**, 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).
8. **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).

Conferences

1. **A. Ibrahim** and P.-N. Roy, "Path-integral Monte Carlo simulations of solid parahydrogen using many-body interaction potentials", in 38^{th} annual symposium on chemical physics, (poster) (University of Waterloo, Nov. 2024).
2. **A. Ibrahim** and P.-N. Roy, "Many-body potential energy surfaces for parahydrogen, and simulations of solid parahydrogen", in 30^{th} canadian symposium on theoretical and computational chemistry, (poster) (Dalhousie University, July 2024).
3. **A. Ibrahim** and P.-N. Roy, "Creating a neural network-based four-body *ab initio* potential energy surface for parahydrogen", in 37^{th} annual symposium on chemical physics, (poster) (University of Waterloo, Nov. 2023).
4. **A. Ibrahim** and P.-N. Roy, "The effects of three-body interactions in simulations of solid parahydrogen", in 12^{th} triennial congress of the world association of theoretical and computational chemists, (poster) (Vancouver Convention Centre, July 2022).
5. **A. Ibrahim** and P.-N. Roy, "Calculating the equation of state of solid parahydrogen using *ab initio* many-body interaction potentials", in 36^{th} annual symposium on chemical physics, (poster) (University of Waterloo, Nov. 2022).
6. **A. Ibrahim**, L. Wang, T. Halverson, R. J. L. Roy, and P.-N. Roy, "Equation of state and vibrational matrix shift of solid parahydrogen", in 35^{th} annual symposium on chemical physics, (poster) (University of Waterloo, Nov. 2019).
7. **A. Ibrahim**, L. Wang, T. Halverson, R. J. L. Roy, and P.-N. Roy, "Equation of state and first principles prediction of the vibrational matrix shift of solid parahydrogen", in 45^{th} international congress of theoretical chemists of latin expression, (poster) (Concordia University, Aug. 2019).
8. **A. Ibrahim** and F. Marsiglio, "Particles bumping into moats: Similarity of wave function solutions of positive and negative barriers", in Undergraduate summer student poster display, (poster) (University of Alberta, Aug. 2017).
9. **A. Ibrahim** and G. Luke, "Crystal growth of spin ice pyrochlores using a floating-zone furnace", in 56^{th} annual canadian undergraduate physics conference, (poster) (Trent University, Oct. 2015).

Courses

Course Code	Name	Grade	Date
PHYS 701	Quantum Mechanics I	92	Fall 2018
PHYS 704	Statistical Physics I	92	Fall 2018
CHEM 740	Special Topics - Quantum Molecular Dynamics	100	Winter 2019
PHYS 705	Statistical Physics II	99	Fall 2018
CHEM 740	Special Topics - Computational Quantum Chemistry	92	Winter 2020
PHYS 776	Special Topics - Computational Physics	Complete	Winter 2020

Awards and Scholarships

Name	Source	Period Held	Value
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	$ 5000(x3)
Graduate Research Studentship	University of Waterloo	05/2021 – 04/2024	$ 5000(x3)
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