

Junan Lin

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SUMMARY

Experienced researcher in **Quantum Algorithms** and **Machine Learning** with a strong background in algorithm development and mathematical modeling. Experienced in developing computational algorithms to solve complex problems across **quantum computing**, **quantum chemistry**, and **de novo drug discovery**. Proven ability to develop novel methodologies, including reinforcement learning frameworks for molecular generation, eigenstate overlap bound algorithms, and quantum error characterization. Familiar with **high-performance computing** on supercomputers and on GPU-powered workstations. Collaborative and **independent problem solver** with a track record of peer-reviewed publications and interdisciplinary research.

PROJECT HIGHLIGHTS

- **Molecular and Protein Design using State-of-the-Art Deep Learning Frameworks** 2024-2025
 1. Developed [BiRLNN](#), a framework utilizing **Bidirectional RNN** and **Reinforcement Learning** for constrained molecular generation, leveraging LSTMs, SMILES/SELFIES molecular encoding, and RL-based optimization.
 2. Developing deep learning framework for **Antibody Affinity Maturation**, utilizing **Cross-Attention** between **Protein Language Model (PLM)** embeddings and multi-head prediction.
 3. Developing CondGMF, a generative AI framework for conditional ligand design combining **3D Multimodal Autoencoder** and **Diffusion Transformer (DiT)**, utilizing **Flow-Matching** and **Classifier-Free Guidance** to produce designs adapted to protein binding sites.
 4. Collaborated across computational chemistry and AI specialists in a fast-paced environment. Five (5) paper published including one (1) first-authored since initiation of the role.
- **Improving Efficiency of Quantum Algorithms for Quantum Chemistry** 2023-2025
 1. Extensive experience with quantum algorithms including **quantum linear solver** (quantum Lanczos-type algorithms), **quantum eigensolver** (quantum phase estimation), and **Hamiltonian simulation**, for quantum chemistry problems.
 2. Designed and implemented [OverlapAnalyzer](#), a rigorous algorithmic framework for model validation and performance guarantees, demonstrating strong first-principles thinking and research innovation.
 3. Performed high-accuracy, classical electronic structure calculations on **high performance computing cluster** (Scinet Niagara Supercomputer).
 4. Designed a novel algorithm for calculating rigorous bounds on wavefunction overlap using polynomial approximation.
 5. Applied **mathematical techniques** such as Chebyshev expansions and **linear programming** for improved computational efficiency.
- **Algorithm Development for Error Characterization in Quantum Computers** 2019-2021
 1. Developed a novel algorithm to characterize state preparation and measurement (SPAM) errors combining quantum information science and statistical techniques.
 2. Combined algorithmic design with **cycle benchmarking** to derive **rigorous bounds** for SPAM errors.
 3. Applied **probabilistic modeling** and **variance estimation** methods to analyze the uncertainty of random variables.
 4. Formulated and proved mathematical bounds, implemented Python-based simulations to simulate algorithmic performance and run experiments on **quantum hardware**.
 5. Papers published on competitive venues including [New Journal of Physics](#), [Physical Review Research](#), [Physical Review A](#), [Physical Review A](#).

EXPERIENCES

- **Research Officer**, National Research Council Canada (Supervisor: Dr. James H.K. Ooi) 2024/01 - Present
- **Postdoctoral Fellow**, University of Toronto, Toronto (Supervisor: Dr. Artur F. Izmaylov) 2023/08 - 2024/01
- **Ph.D. in Physics - Quantum Information**, University of Waterloo (Supervisor: Dr. Raymond Laflamme) 2018/09 - 2023/05
Dissertation: Representation, Characterization, and Mitigation of Noise in Quantum Processors
- **M.Sc. in Physics - Quantum Information**, University of Waterloo (Supervisor: Dr. Raymond Laflamme) 2016/09 - 2018/08
Dissertation: Representing and Probing Errors in Quantum Information Processing Devices
- **B.Sc. in Honours Physics & Chemistry**, McGill University (GPA: 3.96/4) 2012/09 - 2016/04

SELECTED PUBLICATIONS (*= FIRST OR CO-FIRST AUTHOR)

1. Hang Hu, Hsu Kiang Ooi, Mohammad S Ghaemi, **Junan Lin**, Jiří Hostaš, Boniface Yogendran, Anguang Hu, “Mode-Resolved Electron-Phonon Fingerprints Map Topological Protection in Lithium Beyond Born-Oppenheimer”, accepted by *Journal of Physics: Condensed Matter* (2026)
2. *Hang Hu, Jiří Hostaš, Mohammad Sajjad Ghaemi, **Junan Lin**, Shiliang Wang, Anguang Hu, Hsu Kiang Ooi, “Organophosphate Ethyl Paraoxon on Ag and Au Surfaces: A Density Functional Theory Perspective”, accepted by *Physical Chemistry Chemical Physics* (2026)
3. ***Junan Lin**, Mohammad Sajjad Ghaemi, Jiří Hostaš, Anguang Hu, Hang Hu, Hsu Kiang Ooi, “Bidirectional reinforcement learning neural network for constrained molecular design”, *Scientific Reports* 16, 3393 (2026)
4. Hang Hu, Hsu Kiang Ooi, Mohammad S Ghaemi, **Junan Lin**, Jiří Hostaš, Anguang Hu, “Topologically protected quantum metallic bonding of alkali metals: From entangled electron-phonon dynamics”, *APL Quantum* 2, 046111 (2025)
5. *Jiří Hostaš, Mohammad Sajjad Ghaemi, Anguang Hu, Hang Hu, **Junan Lin**, Hsu Kiang Ooi, “VNFlow: Integration of Variational Autoencoders and Normalizing Flows for Novel Molecular Design”, *J Cheminform* 17, 161 (2025)
6. ***Junan Lin**, Artur F. Izmaylov, “Bounds on a Wavefunction Overlap with Hamiltonian Eigen-states: Performance Guarantees for the Quantum Phase Estimation Algorithm”, *arXiv:2503.12224* (2025)
7. ***Junan Lin**, *Nayeli Azucena Rodríguez-Briones, Eduardo Martín-Martínez, Raymond Laflamme, “Thermodynamic Analysis of Algorithmic Cooling Protocols: Efficiency Metrics and Improved Designs”, *Physical Review A* 110, 022215 (2024)
8. Raymond Laflamme, ***Junan Lin**, Tal Mor, “Algorithmic cooling for resolving state preparation and measurement errors in quantum computing”, *Physical Review A* 106 (1), 012439 (2022)
9. *Ningping Cao, ***Junan Lin**, David Kribs, Yiu-Tung Poon, Bei Zeng, Raymond Laflamme, “NISQ: Error correction, mitigation, and noise simulation”, *arXiv:2111.02345* (2021)
10. ***Junan Lin**, Tal Mor, Roman Shapira, “Quantum information and beyond – with quantum candies”, *arXiv:2110.01402* (2021)
11. ***Junan Lin**, Joel J Wallman, Ian Hincks, Raymond Laflamme, “Independent state and measurement characterization for quantum computers”, *Physical Review Research*, 3 (3), 033285 (2021)
12. ***Junan Lin**, Tal Mor, “Quantum Candies and Quantum Cryptography”, *TPNC 2020: Theory and Practice of Natural Computing*, pp. 69-81 (2020)
13. ***Junan Lin**, *Brandon Buonacorsi, Raymond Laflamme, Joel J Wallman, “On the freedom in representing quantum operations”, *New Journal of Physics*, 21(2), 023006 (2019)
14. *Viktorija Glembockyte, **Junan Lin**, Gonzalo Cosa, “Improving the Photostability of Red- and Green-Emissive Single-Molecule Fluorophores via Ni^{2+} Mediated Excited Triplet-State Quenching”, *The Journal of Physical Chemistry B*, 120(46), 11923-11929 (2016)

PRESENTATIONS

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| • American Physical Society Global Physics Summit, Anaheim | Mar 2025 |
| • American Physical Society March Meeting, Las Vegas | Mar 2023 |
| • CIFAR QIS conference, Quebec City | Sep 2022 |
| • Quantum Information Processing Conference (QIP), Pasadena | Mar 2022 |
| • American Physical Society March Meeting, Denver | Mar 2020 |
| • Quantum Information Processing Conference (QIP), Shenzhen | Jan 2020 |
| • Institute for Quantum Computing, Waterloo | Oct 2019 |
| • American Physical Society March Meeting, Boston | Mar 2019 |
| • Undergraduate research symposium, McGill University | Aug 2015 |

AWARDS

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| • Postgraduate Scholarships - Doctoral (PGS-D), NSERC Canada | May 2020 |
| • University of Waterloo Graduate Scholarship, University of Waterloo | Apr 2019 |
| • Alexander Graham Bell Canada Graduate Scholarship - Masters, NSERC Canada | Sep 2017 |
| • President’s Graduate Scholarship, University of Waterloo | Sep 2017 |
| • Provost Graduate Scholarship, University of Waterloo | Aug 2016 |
| • Dean’s Honour List, McGill University | May 2016 |

- **R.F. Robertson Award in Physical Chemistry**, *McGill University* *May 2016*
- **Lennox Scholarship in Science**, *McGill University* *Jul 2015*
- **Undergraduate research award**, *NSERC Canada* *May 2015*
- **Science Class of 1965 Scholarship**, *McGill University* *Jul 2014*
- **James McGill Scholarship**, *McGill University* *Aug 2012*

COMMUNITY INVOLVEMENT

- **Journal Reviewer:** [Quantum](#), [Science China Information Sciences](#), [Advanced Quantum Technologies](#)
- **Conference Reviewer:** QIP 2022, [QIP 2023](#), [QIP 2024](#), [QCTIP 2024](#)

VOLUNTEER EXPERIENCE

- **Judge at [Canadian Undergraduate Physics Conference](#)** *Oct 2022*
- **[Organizing Committee](#) at Canadian Association of Physicists** *May 2021*
- **Demonstrator at the [Lumen festival](#) for IQC, University of Waterloo** *Sep 2019*
- **Group leader at [IQC Physics Lab Days](#), University of Waterloo** *Apr 2019*
- **Judge at [Xplore STEM youth conference](#)** *Nov 2018*
- **Team leader at [Let's Talk Science](#), University of Waterloo** *2016-2019*