



**UNIVERSITY OF CALGARY** FACULTY OF SCIENCE Institute for Quantum Science and Technology



To be a world leader in research and education in pure and applied quantum science and technology.



To advance quantum science and technology through interdisciplinary research, teaching, and outreach.

# **KEY FACTS**

17 research groups

15 postdoctoral fellows

78 graduate students

**12** undergraduate students

69 publications in refereed journal and conference proceedings including Nature (1), Physical Review Letters (5), and Nature Communications (1).

**9** invited talks at national and international conference/workshops

8 million dollars in research funds



DIRECTOR'S REPORT	2
MESSAGE FROM THE CHAIR	4
RESEARCH HIGHLIGHTS Research Achievements Awards	5 5 6
KEY PERFORMANCE INDICATORS	8
RESEARCH GROUPS	11
MANAGEMENT & MEMBERSHIP Institute Structure Governance	20 20 21
PUBLICATIONS	25
Refereed Journal Publications (published) Refereed Conference Proceedings Books and Chapters Student Theses Invited Presentations at Workshops/Conferences	25 29 30 30 30
LINKAGE	31
Academic Collaborations Industrial/Non-profit/Government Collaboration Visitors	31 33 34
GRADUATE COURSES	35
SERVICES AND OUTREACH Conferences/Workshops Professional Services Outreach Lectures Media Coverage	<b>36</b> 36 37 38
RESEARCH GRANTS	41
OBJECTIVES FOR NEXT YEAR	43



# **DIRECTOR'S REPORT**

The Institute for Quantum Science and Technology hosts 17 research groups and about 105 academic members including professors, research staff and students. The Institute has four research themes: molecular modelling, nanotechnology, quantum information and computing, and quantum optics, across the four departments of Chemistry, Computer Science, Mathematics and Statistics, and Physics and Astronomy. In recent years, the Institute has effectively expanded to the provincial level through the growth of the Quantum Alberta initiative, which has three sites: the Universities of Alberta, Calgary and Lethbridge. The Institute for Quantum Science and Technology maintains a strong identity in Calgary but also exists as one of three Quantum Alberta branches.

The Institute is pleased to welcome Pierre Kennepohl and Carlo Maria Scandolo as Faculty members. Pierre moved from the University of British Columbia to the University of Calgary Institute for Quantum Science and Technology in 2020. Pierre's main experimental research activities are in electronic structure and bonding, and in X-ray absorption and emission spectroscopy. Carlo Maria joined the Institute under the Faculty of Science Grand Challenge scheme and is now an Assistant Professor. Previously, Carlo Maria was a graduate student at the University of Oxford in Computer Science. His main research is in theoretical guantum information science including guantum resources and quantum foundations.

The Institute for Quantum Science and Technology has enjoyed a successful year of research and training during the 2020/2021 year. Members of the Institute had 69 papers published in refereed journals and proceedings including nine papers appearing in the toptier journals of Nature (1), Physical Review Letters (5), and Nature Communications (3). The Institute attracted 14 new students into quantum graduate studies programs in 2020/2021. Three masters students graduated and five doctoral students completed their degrees. The Institute hosted 15 postdoctoral researchers with six being recipients of national and provincial postdoctoral fellowship including the NSERC Postdoctoral Fellowship (1), the Alberta Innovates Eyes High Postdoctoral Fellowship (3), Killam Postdoctoral Scholar (1), and University of Calgary Vice President Research Catalyst Grant (1). Matthew Mitchell won a Governor General's Gold Medal.

Success of the Institute is underpinned by support for training and infrastructure with especially notable support from the Natural Sciences and Engineering Research Council (NSERC). Quantum activity is advanced significantly by a Canada Foundation for Innovation (CFI) grant for quantum technology, led by the University of Calgary. The Institute is home to the Alberta Government's Ministry of Job, Economy and Innovation's Major Innovation Fund, which supports quantum science and technology at the Universities of Calgary, Alberta and Lethbridge. This provincial



funding supports 24 graduate students and six postdoctoral researchers at the University of Calgary.

The Institute continues to fulfill its mission as a Faculty of Science Institute and deliver outcomes matching Faculty expectations with respect to the Grand Challenge of "Unlocking Our Digital Future". Furthermore, the Institute has a provincial leadership role through the *Quantum Alberta* initiative, which brings together the province's quantum science and technology researchers under the umbrella of one consortium. As quantum research and development ramps up in Canada and globally, the Institute has a key role to play in ensuring that Calgary continues to be strong on the world stage for quantum science and technology.

#### **Barry C. Sanders**

Director



# **MESSAGE FROM** THE CHAIR

Calgary's economic future is getting brighter because tech start-ups and global companies are establishing a new quantum hub, right here. From nanotechnology and artificial intelligence to quantum internet and biomedical engineering -Calgary is becoming a true quantum capital city.

Through the Institute for Quantum Science and Technology and Quantum Alberta, UCalgary Faculty of Science researchers are also helping continue to drive Canada's global leadership in guantum science and technology.

The 2020-21 Annual Report highlights how the Institute for Quantum Science and Technology is at the forefront of making great strides towards achieving Faculty of Science and UCalgary goals for a digital future. We are proud to have IQST as one of the research leaders in the Faculty of Science and congratulate them on another highly successful year.

#### This year's highlights

1. IQST members vied successfully for two Canada Foundation for Innovation (CFI) grants. Paul Barclay is a lead investigator of the CFI project "A quantum diamond and hybrid photonics foundry". This project will lead to infrastructure that will

support and sustain world-class research into quantum technologies. Tim Friesen and Rob Thompson are the University of Calgary partners in a two-university CFI led by the University of British Columbia. This CFI is HAICU, which stands for Hydrogen Antihydrogen Infrastructure at Canadian Universities, and pursues for quantum innovations in antimatter science.

- 2. IQST welcomed two new members: Pierre Kennepohl (Chemistry) and Carlo Maria Scandolo (Mathematics and Statistics).
- 3. Matthew Mitchell won the Governor General's Gold Medal (Doctoral) in 2020.
- 4. Mphasis, an information technology solution provider specializing in cloud and cognitive services, will set up its Canadian headquarters in Calgary. A strategic partnership with Government of Alberta and the University of Calgary was announced. Establishment of a Quantum City Centre of Excellence (CoE) is to strengthen the UCalgary innovation ecosystem by creating a hub for companies focused on the commercial development of quantum technologies.

Bernhard Mayer Interim Dean, Chair, Board of Directors



# **RESEARCH HIGHLIGHTS**

### **Research Achievements**

The Institute for Quantum Science and Technology (IQST) has significant research achievements over the past year. The following exposition of achievements provides a sample of the kinds of activities and breakthroughs seen within IQST.

Paul Barclay's group had two significant results in the past year, both reported in *Nature Communications*. The first result, involving collaboration with Barry Sanders, reports experimental two-colour interferometry that was demonstrated along with a switching mechanism achieved via exciting an optomechanical dark mode. The second result demonstrates light processing with an optically tunable mechanical memory and specifically extends memory decay time by an order of magnitude, significantly reduces mechanical dissipation and imparts a deterministic large phase shift on stored light.

Gilad Gour's group proves in a *Physical Review Letters* article, that symmetric informationally complete positive operator-valued measures have to satisfy three conditions, in addition to being informationally complete, and note that the oft-overlooked third condition cannot be removed from the other conditions. Gour and Carlo Maria Scandolo together establish computable measures of entanglement between channels, in *Physical Review Letters*, and discover a family of dynamical entanglement measures that provide necessary and sufficient conditions for bipartite channel simulation under local operations and classical communication and under operations with positive partial transpose. In another *Physical Review Letters* article, which is listed as a prestigious Editor's suggestion, Scandolo and collaborators develop an operational resource theory of imaginarily associated with the role of complex numbers in quantum mechanics.

Rob Thompson and Tim Friesen work on the Antihydrogen Laser Physics Apparatus, known as ALPHA, at the European Organization for Nuclear Research (CERN). This past year, their ground-breaking laser cooling of antihydrogen atoms was featured on the cover of *Nature* in March 2021.

Christoph Simon and collaborators carefully studied Hong-Ou-Mandel Interference with imperfect single-photon sources. Their *Physical Review Letters* article explores how unwanted

multiphoton contributions affect interference compared to the case for ideal single-photon sources and apply their approach to quantumdot single-photon sources to access the mean wave-packet overlap of the single-photon component. Simon and other collaborators wrote an insightful article on the emerging commercial landscape for quantum computing; this article was published in *Nature Reviews Physics*.

Inspired by the radical-pair mechanism in cryptochrome associated with avian magnetoreception, Christoph Simon and Dennis Salahub propose, in a *Scientific Reports* article, that xenon nuclear spin influences recombination dynamics of a naturally occurring radical pair of electrons. Their model could explain observed isotopic dependence of the potency of xenon as a general anesthetic and could indicate that radical electron pairs with entangled spin are crucial for consciousness.

Shabir Barzanjeh is lead author of a *Science Advances* article on microwave quantum illumination using a digital receiver. They generate entangled fields to illuminate a room-temperature object at a distance of one metre and implement a digital phaseconjugate receiver based on linear quadrature measurements in a free-space setup. Their scheme outperforms symmetric classical- noise radar under the same conditions, despite the signal path experiencing entanglement breaking.

Barry Sanders collaborated on the first experiment that clones quantum entanglement. Quantum cloning is a famous, purely quantum restriction on copying states, and this experiment, reported in *Physical Review Letters*, demonstrates quantum cloning of two-photon entangled states for the first time with the fidelities of both cloned states having fidelities exceeding one-half.

### Awards

#### International Awards

#### SPIE Optics and Photonics Education Scholarship

Kimberley Ann Owen

#### NATIONAL AWARDS

#### MITACS Globalink Research Award

Shudipto Kazi Amin

Sabari Sekhar

#### Mitacs-Accelerate Graduate Research Internship Program

Seyed Shakib Vedaie

#### NSERC Canada Graduate Scholarships -Doctoral

Joseph Zsombor-Pindera

#### NSERC Canada Graduate Scholarships – Master's Program

Linh Ly

#### NSERC Postdoctoral Fellowship

Maryam Taheri

#### NSERC USRA

Owen Doty

Chris Gergess

#### NSERC Vanier Scholarship

Williams Miranda Delgado

#### Nova Chemicals Graduate Scholarship

Rishabh Shukla

Oliver Calderon

#### Provincial Awards

#### Alberta Graduate Excellence Scholarship

Xining Chen Alison Fulton Kimberley Ann Owen Rishabh Shukla Zhan Yu

#### Alberta Innovates Graduate Students Scholarship

Bishnu Behera Williams Miranda Delgado Salini Karuvad Janet Leahy University of Calgary Awards

#### Alberta Innovates Eyes High Postdoctoral Fellowship

Asha Yadav Hanif Khan Joseph Losby

Bettina Bahlsen Memorial Graduate Scholarship Meryuert Kudaibergenova

Canadian Queen Elizabeth II Diamond Jubilee Scholarships (Advanced Scholars) Nehad AttaElmanan AbdElrahim Mabrouk Department of Biological Science Performance Award Luis Alvarez

Eyes High Doctoral Recruitment Scholarship

Mario Ernesto Valdes Tresanco

Governor General's Gold Medal (Doctoral) Matthew Mitchell

Killam Postdoctoral Scholars Abhijeet Alase

Provost's Doctoral Scholarship Shudipto Kazi Amin

7

VPR Catalyst Grant Martin Schon



# **KEY PERFORMANCE INDICATORS**

# Graduate Student Enrolment and Quality of Entrants



# Publications And Presentations (Highlighted Portion With IQST Student)



### External Awards (Chairs, Fellowships And Scholarships)



### Trainee Destinations After IQST



# Visitors





# **RESEARCH GROUPS**



#### NANOSCALE OPTICS

Explores interactions between light and nanoscale systems such as single atoms, electron spins and nanomechanical structures. Employs nanofabrication methods to engineer optical properties of these systems in order to enhance light-matter coupling. The current focus couples single quantum emitters, or "artificial atoms", to optical nanocavities. The labs are at the University of Calgary and at the NRC National Institute for Nanotechnology in Edmonton, which has advanced nanofabrication tools plus leading quantum optics and nanotechnology researchers.



# INTEGRATED HYBRID QUANTUM CIRCUITS

Focuses on the reversible quantum interface between the superconducting circuits and quantum optical systems. In our lab we develops quantum communication technology that is integrable with superconducting processors for building large-scale quantum networks.



# Dr. Timothy Friesen

#### PRACTICAL QUANTUM COMPUTATION

Focuses on understanding intrinsic properties of physical systems, such as ultracold atomic gases or spin lattices, can be employed to construct larger devices able to perform quantum computation. In addition, the group explores alternative models for the implementation of quantum logic, such as one-way quantum computation, quantum walks, and topological quantum computation.

# TESTING OF FUNDAMENTAL SYMMETRIES WITH ANTIMATTER

Experimental testing of symmetries between matter and antimatter primarily through study of (anti)hydrogen in collaboration with the ALPHA (Antihydrogen Laser Physics Apparatus) experiment at CERN. We focus on the development of particle traps, microwave techniques, and annihilation detection for highprecision spectroscopy and gravitational mass measurements on antihydrogen.



#### QUANTUM INFORMATION THEORY

Employs sophisticated mathematical methods, such as algebraic geometry, matrix analysis, group theory and C\*-algebras, to solve core problems in quantum information science.



#### QUANTUM COMPUTING

Explores the potential powers of quantum systems to develop quantum algorithms, quantum communication protocols, quantum cryptographic protocols, and quantum computer simulations of quantum mechanical systems. Characterizes the powers and their limitations by studying quantum complexity theory, non-locality, entanglement, and quantum information theory.





#### MOLECULAR AND MATERIALS ELECTRONIC STRUCTURE

Explore the relationship between electronic structure of molecules and materials and their broader chemical properties and study the use of such interactions in molecular electronics and other applications. X-ray spectroscopies are the major tools for our exploration of electronic structure.

#### MOLECULAR SIMULATIONS OF LIQUIDS & SOLUTIONS, INTERFACES AND CRYSTALLIZATION

Molecular simulations to examine collections of molecules representing solid or liquid systems. Probes the molecular behaviour to understand properties of liquids and solids and their transformations including nucleation and crystallization. Explores behaviour of the hydroxyl radical in various aqueous environments. Applications range from atmospheric and materials sciences to molecular biology and water treatment.



#### SPECTROSCOPY OF HYDROCARBONS AND MOLECULAR CLUSTERS AND COMPLEXES

Measures forces responsible for formation of atomic and molecular clusters. Investigates the intermolecular potential in the region of the potential minimum. Explores non-additive effects on the interaction energy and to determine possible condensation pathways. Relevant to a range of applications from atmospheric chemistry to molecular biology.



#### QUANTUM CLOUD LAB

Develops experimental capabilities that will lead to practical implementations of quantum links forming the basis of quantum networks that connect distant quantum devices.Research into quantum-key distribution over fibre and freespace channels, non-classical light sources, and quantum memory based on solid-state materials such as rare-earth ion doped crystals.



#### MULTISCALE MODELING OF (BIO) CHEMICAL REACTIONS IN COMPLEX ENVIRONMENTS

Investigates mechanisms and rates of chemical reactions occurring in complex environments. Models enzymatic catalysis, electron transfer between proteins and/or heavy oil upgrading. Employs multiple techniques, from quantum chemistry, to molecular dynamics, to stochastic network analysis, are brought to bear on the problem in the context of high performance computing.



#### QUANTUM INFORMATION SCIENCE

Develops quantum information technologies that have transformative applications and will be feasible within a decade. The research program is divided into five strands: (i) longdistance secure communication, (ii) simulations of complex systems, (iii) implementations of quantum information tasks, (iv) empirical characterization of quantum states and processes, and (v) determining and quantifying all resources for quantum information processing.



# QUANTUM INFORMATION AND FOUNDATIONS

Uses mathematical tools, such as matrix and convex analysis, to quantify quantum resources and optimize their use in information-theoretic protocols. Applies informational methods to foundational problems in quantum theory, especially using the framework of general probabilistic theories, which combine convex analysis with categorical methods.



#### CHEMICAL VAPOR DEPOSITION CHEMISTRY

Focuses on chemical and physical processes underpinning the formation of silicon-containing semiconductor thin film materials using hot-wire chemical vapour deposition. Applies technically demanding laser ionization mass spectrometric and laser spectroscopic techniques to investigate this process at the molecular level. Explores gas- phase reaction chemistry in the formation of silicon carbide and silicon nitride and laser spectroscopy of silicon carbide clusters generated using pulsed discharge and laser ablation methods. Applications include superior-quality films for industrial applications.



#### THEORETICAL QUANTUM OPTICS

Applies unique quantum phenomena such as superposition and entanglement (e.g. a future "quantum internet"), to probe whether these phenomena are universal, and to investigate whether they could play a role in biology (e.g. in neuroscience).



#### TRAPPED ION PHYSICS WITH ATOMS, MOLECULES, AND EXOTIC SPECIES

Develops and measures low-density trapped atoms, molecules and exotic species, especially anti-matter Hydrogen. Collaboration with the Antihydrogen Laser Physics Apparatus (ALPHA) project at CERN involving 40 scientists across 16 institutions. Collaborates with TRIUMF's Ion Trap for Atomic and Nuclear (TITAN) Science, particularly on sympathetic and evaporative cooling.



#### NANOSCALE MATERIAL

Investigates the synthesis, characterization, and structure-property relationships in inorganic solid-state nanomaterial, such as metal-oxide thin films and multimetallic nanoparticles. Develops high-performance materials in technologically and commercially relevant focus areas such as clean-energy conversion and spin-based electronics. Characterizes materials using state- of-the-art methods, such as electrochemical testing, electron microscopy, x-ray diffraction,

and magnetometry based on superconducting quantum interference devices. Properties are analyzed to provide feedback for synthetic approaches for improvement.



# **MANAGEMENT & MEMBERSHIP**

### Institute structure

The Institute is managed on a day-to-day level by the Institute Director and the Institute Administrator. The Director reports to the Board of Directors and is ex officio a member of this Board. The Board reports to the Dean of Faculty of Science who chairs the Board.

The Director and the Administrator of the Institute work on day-to-day matters of the Institute. The Institute Executive comprises the Director, Administrator and three faculty members other than the Director. The Executive meets periodically to discuss and make decisions on executive matters. The Executive receives advice and guidance from the IQST Council, which comprises all full and affiliate faculty members of the Institute and meets three times annually.

All of the Institute's research, teaching, service and outreach activities are conducted by faculty members and their research groups.



### Governance BOARD OF DIRECTORS

#### **Bernhard Mayer**

Interim Dean, Faculty of Science, University of Calgary

#### Marie D'Iorio

Chief Operating Officer, University of Ottawa

#### **Chip Elliott**

Chief Technology Officer (retired) Raytheon BBN Technologies

#### Sir Peter Knight

Senior Fellow in Residence, The Kavli Royal Society International Centre

#### Barry C. Sanders

Professor, Department of Physics and Astronomy, University of Calgary

#### **Carl Williams**

Deputy Director, Physical Measurement Laboratory (PML), National Institute of Standards and Technology (NIST)

#### EXECUTIVE COMMITTEE

#### Paul E. Barclay

Associate Professor, Department of Physics and Astronomy, University of Calgary

#### Peter Kusalik

Professor, Department of Chemistry, University of Calgary

#### **Daniel Oblak**

Assistant Professor, Department of Physics and Astronomy, University of Calgary

#### Barry C. Sanders

Professor, Department of Physics and Astronomy, University of Calgary

#### COUNCIL

#### Faculty Members

#### **Paul Barclay**

Associate Professor, Department of Physics and Astronomy, University of Calgary

#### Shabir Barzanjeh

Assistant Professor. Department of Physics and Astronomy, University of Calgary

#### **David Feder**

Associate Professor, Department of Physics and Astronomy, University of Calgary

#### **Timothy Friesen**

Assistant Professor. Department of Physics and Astronomy, University of Calgary

#### **Gilad Gour**

Professor, Department of Mathematics and Statistics, University of Calgary

#### Peter Høyer

Associate Professor, Department of Computer Science, University of Calgary

#### **Kierre Kennepohl**

Associate Professor, Department of Chemistry, University of Calgary

#### Peter Kusalik

Professor, Department of Chemistry, University of Calgary

#### Nasser Moazzen-Ahmadi

Professor, Department of Physics and Astronomy, University of Calgary

#### Daniel Oblak

Assistant Professor

Department of Physics and Astronomy, University of Calgary

#### Dennis Salahub

Professor Emeritus, Department of Chemistry, University of Calgary

#### Barry C. Sanders

Professor, Department of Physics and Astronomy, University of Calgary

#### Carlo Maria Scandolo

Assistant Professor, Department of Mathematics and Statistics, University of Calgary

#### Yujun Shi

Professor, Department of Chemistry, University of Calgary

#### **Christoph Simon**

Professor, Department of Physics and Astronomy, University of Calgary

#### **Robert I. Thompson**

Professor, Department of Physics and Astronomy, University of Calgary

#### Simon Trudel

Associate Professor, Department of Chemistry, University of Calgary

#### Affiliate Members

#### Robin Cockett

Professor, Department of Computer Science, University of Calgary

#### David Hobill

Professor Emeritus Department of Physics and Astronomy, University of Calgary

#### Sergei Noskov

Professor, Department of Biological Sciences, University of Calgary

#### **Reginald Paul**

Professor, Department of Chemistry, University of Calgary

#### Rei Safavi-Naini

Professor, Department of Computer Science, University of Calgary

#### **Renate Scheidler**

Professor, Department of Mathematics and Statistics, University of Calgary

#### **Peter Tieleman**

Professor, Department of Biological Sciences, University of Calgary

#### **Daniel Trad**

Associate Professor, Department of Geoscience, University of Calgary

#### **Richard Zach**

Professor, Department of Philosophy, University of Calgary

#### Postdoctoral Fellows

Abhijeet Alase Morteza Chehel Amirani (completed March 2021→research associate, University of Calgary) Rogelio Delgado Venegas Ghazal Hajisalem (completed November 2020→research associate, University of Victoria) Vinaya Kumar Kavatamane Rathnakara Faezeh Kimiaee Asadi Sourabh Kumar David Lake (completed June 2020→postdoc, California Institute of Technology) Joseph Losby Trong Huynh Buu Ngo Nicholas Randell Carlo Maria Scandolo (completed August 2020→assistant professor, University of Calgary) Martin Schon Denis Sukachev Maryam Taheri Research Associates/Coordinators/ Engineers

Roohollah Ghobadi (research associate) Erhan Saglamyurek (research associate) Hristina Zhekova (staff scientist) Rana Zibakhsh Shabgahi (research assistant)

#### Graduate Students (PhD Program)

David Amaro Alcalá Shudipto Kazi Amin Behnam Ashrafkhani Mohsen Bagherimehrab Aaron Barclay Bishnupada Behera

Stephanie Bovincini Oliver Calderon Archismita Dalal Katelynn Daly Balarama Sridhar Dwadasi Carlos Enriquez-Victorero Andrew Evans Alison Fulton (graduated August 2020→researcher, Tommy Gun's) Victor Arturo Mora Gomez Sumit Goswami Masoud Habibi Davijani Lizandra Barrios Herrera Jiawei Ji Hamidreza Kaviani (graduated September 2020) Faezeh Kimiaee Asadi (graduated September 2020→postdoc, University of Calgary) Sourabh Kumar (graduated August 2020 $\rightarrow$ postdoc, University of Calgary) Prasoon Kumar Shandilya Salini Karuvade Pascal Lefebvre Nehad AttaElmanan AbdElrahim Mabrouk Williams Miranda Delgado Mahmood Noweir Eduardo Paez Adam Powell Rishabh Gaurav Saxena **Rishabh Shukla** Shahrzad Taherizadegan Seved Shakib Vedaie

Stephen Wein (graduated March 2021→postdoc, Institut Néel in Grenoble, France) Hadi Zadeh Haghighi Parisa Zarkeshian Joseph Zsombor-Pindera

#### Graduate Students (MSc Program)

Omid Aligholamioskooee Mustafa Amin Aradhana Anil Ashkan Bayat Dante Renato Bencivenga Parisa Behjat Khatouni Fasiha Binat Zafar Xining Chen Anustup Das **Travis Gartner Jianing Geng** Thomas Hujon Santiago Jimenez Pirouz Kiani Mojtaba Komeili Murali Krishna Kurmapu (graduated November 2020→researcher, 1QBit) Janet Leahy Pengcheng Liao Zhuohao(Ray) Liu Linh Ly Xinyuan Ma Blaine Jeffrey McLaughlin **Robert Riley Nerem** 

Joan Ngure Yasser Novo-Fernández Kimberlev Ann Owen Nihari Sathsarani Pathirannehe Kuntal Sengupta (graduated September 2020→PhD, University of York) Sara Shafiei Alavijeh Kenneth Sharman Jordan Smith Armin Tabesh Praveen Wakwella Taozhe (Evan) Wu Yufeng Wu (graduated August 2020→PhD, Yale University) Yanjuan Xiong Zhan Yu Elham Zohari

#### Undergraduate Students

Benjamin Appleyard (UofC PHYS598) Rhett Bryant (UofC CHEM402) Breanna Collins (UofC summer student) Owen Doty (NSERC USRA & UofC PHYS598) Chris Gergess (NSERC USRA & thesis project of Mount Royal University) Sye Ghebretnsae (UofC PHYS598) Taylor Kergan (UofC PHYS598) Anna Marie Lewrenz (UofC CHEM502) Sabari Sekhar (MITACS Globalink) Kenneth Sharman (UofC PHYS 598) Amit Shalev (UofC PHYS598) Jordan Smith (UofC PHYS 598)

#### Administration

Xining Chen (Part-time Webmaster) Jing (Nancy) Lu (Administrator)



# PUBLICATIONS

### Refereed Journal Publications (published)

K. S. Amin, X.-J. Hu, D. R. Salahub, C. Baldauf, C. Lim and S. Y. Noskov, "Benchmarking polarizable and non-polarizable force fields for Ca<sup>2+</sup>-peptides against a comprehensive QM dataset", *Journal of Chemical Physics* **153**(14): 144102 (16 pp.), October 2020.

G. Arnold, M. Wulf, S. Barzanjeh, E. S. Redchenko, A. Rueda, W. J. Hease, F. Hassani and J. M. Fink, "Converting microwave and telecom photons with a silicon photonic nanomechanical interface", *Nature Communications* **11**: 4460 (7 pp.), September 2020.

S. Asgarnezhad-Zorgabad and B. C. Sanders, "Nonlinear frequency conversions via weak surface polaritonic wave breaking in a hybrid plasmonic waveguide", *Optics Letters* **45**(19): 5432–5435, September 2020.

C. J. Baker, W. A. Bertsche, A. Capra,
C. Carruth, C. L. Cesar, M. Charlton, A.
Christensen, R. Collister, A. Cridland Mathad,
S. Eriksson, A. Evans, N. Evetts, J. Fajans,
T. Friesen, M. C. Fujiwara, D. R. Gill, P.
Grandemange, P. Granum, J. S. Hangst, W.
N. Hardy, M. E. Hayden, D. Hodgkinson, E.
Hunter, C. A. Isaac, M. A. Johnson, J. M.

Jones, S. A. Jones, S. Jonsell, A. Khramov, P. Knapp, L. Kurchaninov, N. Madsen, D. Maxwell, J. T. K. McKenna, S. Menary, J. M. Michan, T. Momose, P. S. Mullan, J. J. Munich, K. Olchanski, A. Olin, J. Peszka, A. Powell, P. Pusa, C. Ø. Rasmussen, F. Robicheaux, R. L. Sacramento, M. Sameed, E. Sarid, D. M. Silveira, D. M. Starko, C. So, G. Stutter, T. D. Tharp, A. Thibeault, R. I. Thompson, D. P. Van Der Werf and J. S. Wurtele, "Laser cooling of antihydrogen atoms", *Nature* **592**: 35–42, March 2021.

A. J. Barclay, A. R. W. McKellar and N. Moazzen-Ahmadi, "Spectra of  $CO_2-N_2$  dimer in the 4.2 µm region: Symmetry breaking of the intramolecular  $CO_2$  bend, the intermolecular bend, and higher K-values for the fundamental", *Journal of Chemical Physics* **153**(1): 014303 (7 pp.), July 2020.

A. J. Barclay, A. P. Charmet, A. R. W. McKellar and N. Moazzen-Ahmadi, "Exploring the next step in micro-solvation of CO in water: Infrared spectra and structural calculations of  $(H_2O)_4$ -CO and  $(D_2O)_4$ -CO", *Journal of Chemical Physics* **154**(4): 044310 (7 pp.), January 2021. J. Burniston, M. Grabowecky, C. M. Scandolo, G. Chiribella and G. Gour, "Necessary and sufficient conditions on measurements of quantum channels", *Proceedings of The Royal Society of London Series A. Mathematical, Physical and Engineering Sciences* **476**(2236): 20190832 (10 pp.), 29 April 2020.

R. Chatterjee, K. Joarder, S. Chatterjee, B. C. Sanders and U. Sinha, "qkdSIM, a simulation toolkit for quantum key distribution including imperfections: Performance analysis and demonstration of the B92 protocol using heralded photons", *Physical Review Applied* **14**(02): 024036 (64 pp.), August 2020.

E. Chitambar, J. I. de Vicente, M. W. Girard and G. Gour, "Entanglement manipulation beyond local operations and classical communication", *Journal of Mathematical Physics* **61**(4): 042201 (25 pp.), April 2020.

Y.-Y. Chu, A. C. Kaushik, X.-G. Wang, W. Wang, Y.-F. Zhang, X.-Q. Shan, D. R. Salahub, Y. Xiong and D.-Q. Wei, "DTI-CDF: a cascade deep forest model towards the prediction of drug-target interactions based on hybrid features", *Briefings in Bioinformatics* **22**(1): 451–462, January 2021.

D. Dalacu, D. B. Northeast, P. J. Poole, G. C. Aers, R. L. Williams, K. A. Owen and D. Oblak, "Pump power control of photon statistics in a nanowire quantum dot", *Physical Review A* **102**(11): 115401 (7 pp.), September 2020.

A. Dash, B. Blasiak, B. Tomanek, A. Banerjee, S. Trudel, P. Latta and F. C. J. M. van Veggel, "Colloidally stable monodisperse fe nanoparticles as  $T_2$  Contrast agents for highfield clinical and preclinical magnetic resonance imaging", ACS Applied Nano Materials **4**(2): 1235–1242, February 2021.

J. Davidson, J. Lefebvre, J. Zhang, D. Oblak and W. Tittel, "Improved light-matter interaction for storage of quantum states of light in a thulium-doped crystal cavity", *Physical Review A* **101**(4): 042333 (5 pp.), April 2020. P. C. Dong, E. A. Fisher, M.-Vicki Meli and S. Trudel, "Tuning the magnetism of gold nanoparticles by changing the thiol coating", *Nanoscale* **12**(38): 19797–19803, September 2020.

K. R. Fast, J. A. Thibault, V. T. K. Sauer, M.
G. Dunsmore, A. Kav, J. E. Losby, Z. Diao,
E. J. Luber, M. Belov and M. R. Freeman,
"Simultaneous three-axis torque measurements of micromagnetism", *AIP Advances* **11**(1): 015119 (5 pp.), January 2021.

B. R. L. Galvão, L. P. Viegas, D. R. Salahub and M. P. Lourenço, "Reliability of semiempirical and DFTB methods for the global optimization of the structures of nanoclusters", *Journal of Molecular Modeling* **26**: 303 (8 pp.), October 2020.

T. A. Gartner, A. J. Barclay, A. R. W. McKellar and N. Moazzen-Ahmadi, "Symmetry breaking of the bending mode of CO2 in the presence of Ar", *Physical Chemistry Chemical Physics* **22**: 21488–21493, September 2020.

I. J. Geng, K. Golubeva and G. Gour, "What are the minimal conditions required to define a symmetric informationally complete generalized measurement?", *Physical Review Letters* **126**(10): 100401 (5 pp.), March 2021.

M. R. Ghaani, P. G. Kusalik and N. J. English, "Massive generation of metastable bulk nanobubbles in water by external electric fields", *Science Advances* **6**(14): eaaz0094, April 2020.

G. Gour and C. M. Scandolo, "Dynamical entanglement", *Physical Review Letters* **125**(18): 180505 (6 pp.), October 2020.

G. Gour and M. Tomamichel, "Optimal extensions of resource measures and their applications", *Physical Review A* **102**(6): 062401 (13 pp.), December 2020.

G. Gour, "Uniqueness and optimality of dynamical extensions of divergences", *PRX Quantum* **2**(1): 010313 (16 pp.), January 2021.

C. A. Horwood, E. Owusu-Ansah, Y. J. Shi and V. I. Birss, "Pulsed laser induced dewetting of Au thin films on Ta2O5 substrates", *Chemical Physics* **541**(11): 110926 (9 pp.), January 2021.

P. Høyer and Z. Yu, "Analysis of lackadaisical quantum walks", *Quantum Information and Computation* **20**(13 & 14): 1138–1153, November 2020.

M. Jafarzadeh, Y.-D. Wu, Y. R. Sanders and B. C. Sanders, "Randomized benchmarking for qudit Clifford gates", *New Journal of Physics* **22**(6): 063014 (10 pp.), June 2020.

H. Kaviani, R. Ghobadi, B. Behera, M. Wu, A. C. Hryciw, S. Vo, D. Fattal and P. E. Barclay, "Optomechanical detection of light with orbital angular momentum", *Optics Express* **28**(10): 15482–15496, May 2020.

A. Khalique, H. de Guise and B. C. Sanders, "Interferometrically estimating a quadratic form for any immanant of a matrix and its permutations", *Physical Review A* **101**(5): 052314 (9 pp.), May 2020.

F. Kimiaee Asadi, S. Wein and C. Simon, "Cavity-assisted controlled phase-flip gates", *Physical Review A* **102**(1): 013703 (14 pp.), July 2020.

F. Kimiaee Asadi, S. Wein and C. Simon, "Protocols for long-distance quantum communication with single <sup>167</sup>Er ions", *Quantum Science and Technology* **5**(4): 045015 (16 pp.), September 2020.

D. Lake, M. J. Mitchell, B. C. Sanders and P. E. Barclay, "Two-colour interferometry and switching through optomechanical dark mode excitation", *Nature Communications* **11**: 2208 (7 pp.), May 2020.

D. Lake, M. J. Mitchell, D. D. Sukachev and P. E. Barclay, "Processing light with an optically tunable mechanical memory", *Nature Communications* **12**: 663 (9 pp.), January 2021.

P. Lefebvre, R. Valivarthi, Q. Zhou, L. Oesterling, D. Oblak and W. Tittel, "Compact energy–time entanglement source using cascaded nonlinear interactions", *Journal of the Optical Society of America B* **38**(4): 1380–1385, March 2021.

H.-B. Liang, Y.-G. Su, X. Xiao, Y.-M Che, B. C. Sanders and X.-G. Wang, "Criticality in two-mode interferometers", *Physical Review A* **102**(1): 013722 (6 pp.), July 2020.

E. R. MacQuarrie, C. Simon, S. Simmons and E. Maine, "The emerging commercial landscape of quantum computing", *Nature Reviews Physics* **2**: 596–598, October 2020.

K. Mori, M. G. Dunsmore, J. E. Losby, D. M. Jenson, M. Belov and M. R. Freeman, "Einsteinde Hass effect at radio frequencies in and near magnetic equilibrium", *Physical Review B* **102**(5): 054415 (13 pp.), August 2020.

A. Munir and B. C. Sanders, "Creating deterministic collisions between two orbiting bodies", *Physical Review A* **102**(4): 043113 (13 pp.), October 2020.

B. Nagarajan, M. A. W. Schoen, S. Trudel, A. J. Qureshi and P. Mertiny, "Rheologyassisted microstructure control for printing magnetic composites—material and process development", *Polymers* **12**(9): 2143 (19 pp.), September 2020. .

M. Noori, S. S. Vedaie, I. Singh, D. Crawford, J. S. Oberoi, B. C. Sanders and E. Zahedinejad, "Analog-quantum feature mapping for machine-learning applications", *Physical Review Applied* **14**(3): 034034 (10 pp.), September 2020.

M. Noweir, M. Helaoui, D. Oblak and F. M. Ghannouchi, "Linearized full duplex radioover-fiber-over-space mixerless transceiver architecture", *IEEE Photonics Technology Letters* **33**(2): 113–116, January 2021.

T. Okbinoglu and P. Kennepohl, "Nature of S-N bonding in sulfonamides and related compounds: Insights into π-bonding contributions from sulfur K-edge X-ray absorption spectroscopy", *Journal of Physical Chemistry A* **125**(2): 615–620, January 2021. H. Ollivier, S. E. Thomas, S. Wein, I. Maillette de Buy Wenniger, N. Coste, J. C. Loredo, N. Somaschi, A. Harouri, A. Lemaitre, I. Sagnes, L. Lanco, C. Simon, C. Anton, O. Krebs and P. Senellart, "Hong-Ou-Mandel interference with imperfect single photon sources", *Physical Review Letters* **126**(6): 063602 (6 pp.), February 2021.

E. Owusu-Ansah, V. I. Birss and Y. J. Shi, "Mechanisms of pulsed laser-induced dewetting of thin platinum films on tantalum substrates—A quantitative study", *Journal of Physical Chemistry C* **124**(42): 23387–23393, September 2020.

L.-C. Peng, D. Wu, H.-S. Zhong, Y.-H. Luo, Y. Li, Y. Hu, X. Jiang, M.-C. Chen, L. Li, N.-L. Liu, K. Nemoto, W. J. Munro, B. C. Sanders, C.-Y. Lu and J.-W. Pan, "Cloning of quantum entanglement", *Physical Review Letters* **125**(21): 210502 (6 pp.), November 2020.

C. Qian, Y.-D. Wu, J.-W. Ji, Y.-L. Xiao and B. C. Sanders, "Multiple uncertainty relation for accelerated quantum information", *Physical Review D* **102**(9): 096009 (9 pp.), November 2020.

M. Saffman, I. I. Beterov, A. Dalal, E. J. Paez and B. C. Sanders, "Symmetric Rydberg controlled-Z gates with adiabatic pulses", *Physical Review A* **101**(6): 062309 (10 pp.), June 2020.

G. Saxena, E. Chitambar and G. Gour, "Dynamical resource theory of quantum coherence", *Physical Review Research* **2**(2): 023298 (27 pp.), June 2020.

M. A. W. Schoen, N. M. Randell, O. Calderon, S. Jimenez Villegas, Z. Thomson, R. Chernikov and S. Trudel, "Structural Evolution in Photodeposited nickel (oxy)hydroxide oxygen evolution electrocatalysts", *ACS Applied Energy Materials* **3**(12): 12407–12416, November 2020.

N. Shukla, S. Nimmrichter and B. C. Sanders, "Squeezed comb states", *Physical Review A* **103**(1): 012408 (9 pp.), January 2021. J. Smith, H. Zadeh Haghighi, D. R. Salahub and C. Simon, "Radical pairs may play a role in xenon-induced general anesthesia", *Scientific Reports* **11**: 6287 (13 pp.), March 2021.

R. Valivarthi, S. I. Davis, C. Peña, S. Xie, N. Lauk, L. Narváez, J. P. Allmaras, A. D. Beyer, Y. Gim, M. Hussein, G. Iskander, H. L. Kim, B. Korzh, A. Mueller, M. Rominsky, M. Shaw, C. Simon, D. Oblak, N. Sinclair and M. Spiropulu, "Teleportation systems toward a quantum internet", *PRX Quantum* **1**(2): 020317 (16 pp.), December 2020.

Y.-C. Wang, Z.-X. Hu, B. C. Sanders and S. Kais, "Qudits and high-dimensional quantum computing", *Frontiers in Physics* **8**: 589504 (24 pp.), November 2020.

S. Wein, J.-W. Ji, Y.-F. Wu, F. Kimiaee Asadi, R. Ghobadi and C. Simon, "Analyzing photon-count heralded entanglement generation between solid-state spin qubits by decomposing the master-equation dynamics", *Physical Review A* **102**(3): 033701 (15 pp.), September 2020.

Y.-F. Wu, J.-L. Liu and C. Simon, "Nearterm performance of quantum repeaters with imperfect ensemble-based quantum memories", *Physical Review A 101*(4): 042301 (14 pp.), April 2020.

K.-D. Wu, T. V. Kondra, S. Rana, C. M. Scandolo, G.-Y. Xiang, C.-F. Li, G.-C. Guo and A. Streltsov, "Operational resource theory of imaginarity", *Physical Review Letters* **126**(9): 090401 (7 pp.), March 2021.

K.-D. Wu, T. V. Kondra, S. Rana, C. M. Scandolo, G.-Y. Xiang, C.-F. Li, G.-C. Guo and A. Streltsov, "Resource theory of imaginarity: Quantification and state conversion", *Physical Review A* **103**(3): 032401 (13 pp.), March 2021.

Q. Xi, S.-H. Wei, C.-Z. Yuan, X.-Y. Zhang, Y. Wang, H.-Z. Song, G.-W. Deng, B. Jing, D. Oblak and Q. Zhou, "Experimental observation of coherent interaction between laser and erbium ions ensemble doped in fiber at sub 10 mK", *Science China Information Sciences* **63**(18): 180505 (7 pp.), July 2020.

Y.-L. Xiao, Y. Xiang, Q.-Y. He and B. C. Sanders, "Quasi-fine-grained uncertainty relations", *New Journal of Physics* **22**(7): 073063 (16 pp.), July 2020.

Z.-C. Zhang, G.-J. Guo, N.-Y. Wu and P. G. Kusalik, "Molecular insights into guest and composition dependence of mixed hydrate nucleation", *Journal of Physical Chemistry C* **124**(45): 25078–25086, October 2020.

J. Zsombor-Pindera, F. Effaty, L. Escomel, B. Patrick, P. Kennepohl and X. Ottenwaelder, "Five nitrogen oxidation states from nitro to amine: Stabilization and reactivity of a metastable arylhydroxylamine complex", *Journal of the American Chemical Society* **142**(45): 19023–19028, October 2020.

### Refereed Conference Proceedings

S. Barzanjeh, S. Pirandola, D. Vitali and J. M. Fink, "Microwave quantum illumination with a digital phase-conjugated receiver", Proceedings of 2020 IEEE Radar Conference (RadarConf20), Florence, Italy, 21–25 September 2020.

B. Behera, H. Kaviani, G. Hajesalem, G. Luiz and P. E. Barclay, "High-frequency photonic crystal torsional optomechanics", STh1R.4, Proceedings of 2020 Conference on Lasers and Electro-Optics (CLEO): Science and Innovations 2020, San Jose, United States of America, 10–15 May 2020.

D. Bencivanga, X. Chen and P. Høyer, "Quantum sampling in Markov chains", Proceedings of 24th Annual Conference on Quantum Information Processing, Munich, Germany, 1–5 February 2021.

A. Dalal, E. J. Paez, S. S. Vedaie and B. C. Sanders, "Machine learning framework for control inclassical and quantum domains", Proceedings of European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning (ESANN 2020), pp. 267–272, virtual, 2–4 October 2020. A. Das, P. K. Shandilya, D. J. Lee, S. Kim, K. Gumin, D. Lake, M. J. Mitchell, I. Aharonovich, J. Park and P. E. Barclay, "Demonstration of hexagonal boron nitride optical microcavities with Q > 200,000", SM4R.1, Proceedings of CLEO: Science and Innovations 2020, Washington DC, United States of America, 10–15 May 2020.

G. Gour and M. Wilde, "Entropy of a quantum channel: Definition, properties, and application", Proceedings of 2020 IEEE International Symposium on Information Theory, Los Angeles, United States of America, 20–26 June 2020.

N. Lauk, R. Valivarthi, S. Davis, L. Narváez, Y. Gim, M. Hussein, G. Iskander, B. Korzh, A. Mueller, D. Oblak, C. Peña, M. Rominsky, M. Shaw, C. Simon, N. Sinclair, P. Spentzouris, M. Spiropulu, D. Tang and S. Xie, "Modeling INQNET's time-bin qubit teleportation experiments using phase space methods", JM6B.27, Proceedings of Laser Science 2020, Washington DC, United States of America, 14–17 September 2020.

P. K. Shandilya, D. Lake, M. J. Mitchell, D. D. Sukachev and P. E. Barclay, "Optomechanical driving of spins", Proceedings of SPIE OPTO: Quantum Computing, Communication, and Simulation (SPIE OPTO 2021), 11699, virtual, 6–12 March 2021.

M. Taheri, B. Zanca, S. Jimenez Villegas, M. Dolgos, S. Bryant and S. Trudel, "Densifying BaTiO3 polycrystalline ceramics without affecting size and ferroelectric properties", Proceedings of 2020 Joint Conference of the IEEE International Frequency Control Symposium and International Symposium on Applications of Ferroelectrics (IFCS-ISAF), virtual, 19–23 July 2020.

R. Valivarthi, S. Davis, L. Narváez, Y. Gim, M. Hussein, G. Iskander, B. Korzh, N. Lauk, A. Mueller, D. Oblak, C. Peña, M. Rominsky, M. Shaw, C. Simon, N. Sinclair, P. Spentzouris, M. Spiropulu, D. Tang and S. Xie, "High-fidelity quantum teleportation of time-bin qubits at telecommunication wavelength ", QTh7A.5, Proceedings of OSA Quantum 2.0, Washington DC, United States of America, 14–17 September 2020.

### **Books and Chapters**

S. B. Dwadasi, K. S. Amin, D. R. Salahub and S. Y. Noskov, "QM/MM Simulations of Proteins: Is Explicit Inclusion of Polarization on the Horizon?", section in book: Multiscale Dynamics Simulations: Nano and Nano-bio Systems in Complex Environments, Dennis R. Salahub & D.-Q. Wei, eds., published by Royal Society of Chemistry London in 2021.

### Student Theses

H. Kaviani, "Cavity optomechanics for nonlinear coupling and torsional sensing" (PhD Thesis), December 2020.

F. Kimiaee Asadi, "Long-distance quantum communication with single solid-state spins" (PhD Thesis), September 2020.

S. Krishna, "Machine learning assisted quantum state tomography" (MSc Thesis), November 2020.

A. J. Fulton, "Nanostructured silicon for lithium ion batteries: From porous silicon to silicon nanowires" (PhD Thesis), August 2020.

S. Kumar, "Photonic aspects of networks: from long-distance quantum networks to the brain" (PhD Thesis), August 2020.

K. Sengupta, "Dynamical Bell nonlocality" (MSc Thesis), September 2020.

S. Wein, "Modelling Markovian light-matter interactions for quantum optical devices in the solid state" (PhD Thesis), March 2021.

Y.-F. Wu, "Near-term quantum repeaters" (MSc Thesis), August 2020.

### Invited Presentations at Workshops/Conferences

26 May 2020, <u>C. Simon</u>, "Entanglement from the quantum internet to quantum neuroscience", Photonics North 2020 (virtual), Niagara Falls, Canada, 26–28 May 2020.

28 May 2020, <u>D. Oblak</u>, J. Davidson, P. Lefebvre, J. Zhang, W. Tittel, C. Simon and B. C. Sanders, "Quantum memory and progress towards quantum networks", Photonics North 2020 (virtual), Niagara Falls, Canada, 26–28 May 2020.

30 June 2020, <u>C. Simon</u>, "Towards the quantum internet", National Research Council (NRC) Quantum Computing Workshop (virtual), 29–30 June 2020.

19 August 2020, <u>C. Simon</u>, "Towards the quantum internet", Quantum-secured Communications for Canada Workshop (virtual), 19 August 2020.

14 September 2020, <u>C. Simon</u>, "Could quantum entanglement help explain consciousness?", The Science of Consciousness 2020 (virtual), 14–18 September 2020.

5 November 2020, <u>B. C. Sanders</u>, "Building a quantum computer", 2020 ACM/IEEE International Workshop on System-Level Interconnect Problems and Pathfinding (SLIP<sup>2</sup>) (virtual), 2–5 November 2020.

6 November 2020, <u>B. C. Sanders</u>, "Security for quantum network" (keynote), 11th IEEE Annual Information Technology, Electronics and Mobile Communication Conference (IEMCON, virtual), 4–7 November 2021.

14 January 2021, <u>C. Simon</u>, "Towards the quantum internet", Quantum Days Conference (virtual), 13–15 January 2021.

6 March 2021, <u>C. Simon</u>, "Near-term quantum repeaters", SPIE Photonics West 2021 (virtual), 6–11 March 2021.



# LINKAGE

# Academic Collaborations

#### International Institutions

Aarhus University, Denmark

Ben-Gurion University of the Negev, Israel

California Institute of Technology, United States of America

Centro de Investigación y de Estudios Avanzados (CINVESTAV), Mexico

Cockcroft Institute, United Kingdom

European Organization for Nuclear Research (CERN), Switzerland

Grand Accélérateur National d'Ions Lourds, France

GSI Helmholtz Centre for Heavy Ion Research, Germany

Harvard University, United States of America

Jagiellonian Univeristy Krakow, Poland

Korean Institute of Science and Technology, South Korea

Imam Abdulrahman Bin Faisal University, Saudi Arabia

Indian Statistical Institute, India

Institute of Science and Technology, Austria

Israel Institute of Technology (Technion), Israel

Massachusetts Institute of Technology (Board Institute), United States of America

National Institutes of Health, United States of America

National Institute for Standards and Technology (Gaithersburg), United States of America

Polish Academy of Sciences, Poland

Politecnico di Milano, Italy

Purdue University, United States of America

Qingdao Institute of Marine Geology, People's Republic of China

Radboud University, the Netherlands

Raman Research Institute, India

Shandong University, People's Republic of China

Shariff University of Technology, Iran

Soreq Nuclear Research Centre, Israel

Stockholm University, Sweden

Swansea University, United Kingdom

Università Ca' Foscari Venezia, Italy

Université catholique de Louvain, Belgium

Université Paris-Saclay, France

Universidade Federal do Espírito Santo, Brazil

Universidade Federal do Rio de Janeiro, Brazil

University College Dublin, Ireland

University of California at Berkeley, United States of America

University of California at Los Angeles, United States of America

University of Chicago, United States of America

University of Electronic Science and Technology of China, People's Republic of China

University of Gdańsk, Poland

University of Manchester, United Kingdom

University of Maryland, United States of America

University of Oxford, United Kingdom

University of Queensland, Australia

University of Science and Technology of China, People's Republic of China

University of Science and Technology, South Korea

University of Technology Sydney, Australia

University of Warsaw, Poland

#### National Institutions

British Columbia Institute of Technology Lakehead University Simon Fraser University Université de Sherbrooke University of Victoria University of Waterloo

# Industrial/Non-profit/Government Collaboration

COLLABORATIVE ENTITY	NAME	ROLE	NATURE			RESEARCH TOPIC
			Collaboration	Service	Training	
1QBit	Seyed Shakib Vedaie	Collaborator (scientific)	×		MITACS graduate internship	Quantum machine learning
ApexQubit	Barry C. Sanders	Scientific Advisory Board Member		×		Quantum Computing
Argonne National Lab	Daniel Oblak	Collaborator	×			Autonomous calibration of quantum networks
Clariant AG	Pierre Kennepohl	Collaborator	×			Rapid in operando spectroscopic characterization of catalysts
Creative Destruction Lab (CDL)	Barry C. Sanders	Mentor		×		Supporting quantum ventures
Jet Propulsion Laboratory	Daniel Oblak	Collaborator	×			Superconducting nano-wire single photon detectors for bio-photon detection
Katal Engergy Inc.	Dennis Salahub & Morteza Chehel Amirani	Researcher	×		×	Extending diesel fuel, molecular dynamic mechanisms
Lumerical	Paul E. Barclay	Collaborator	×			Optomechanical simulation
National Research Council Ottawa	Christoph Simon	Collaborator	×			Quantum memories/ transducers
National Research Council Ottawa	Dennis Salahub, Jiri Hostas & Lizandra Barrios Herrera	Researcher	×		×	Al for design, nanocatalysts
Oxford Instrument	Paul E. Barclay	Collaborator	×			Diamond quantum tech
TRIUMF	Robert I. Thompson & Timothy Friesen	Collaborator	×			ALPHA project

# Visitors

NAME	INSTITUTION
Dorcas Attuabea Addo	Kwame Nkrumah University of Science and Technology
Snehasis Addy	Indian Institute of Technology, Dhanbad
Hessa Muneef Alotaibi	The Public Authority for Applied Education and Training, Kuwait
Karabee Batta	Birla Institute of Technology and Science (BITS Pilani)
Sarah Brandsen	Duke University
Bo Fu	Shandong University
Na Lin	Shandong University
Mosayeb Naseri	Isamic Azad University, Kermanshah Branch
Haleema Sadia Qureshi	COMSATS University, Islamabad
Yi Shen	Beihang University
Shakir Ullah	COMSATS University, Islamabad
Siren Yang	Dalian University of Technology


# **GRADUATE COURSES**

### University of Calgary

COURSE NAME	INSTRUCTOR	DESCRIPTION
PHYS615 Non-Relativistic Quantum Mechanics	P. E. Barclay	Mathematical formalism of quantum mechanics. Topics may include addition of angular momenta, Clebsch-Gordan coefficients, Wigner-Eckart theorem; charged particles in electric and magnetic fields; quantum operators; approximation methods; scattering; quantum nonlocality, Einstein-Podolsky-Rosen paradox, Bell's theorem.
CPSC619 Introduction to Quantum Computing	P. Høyer	Introduction to quantum computing. Quantum algorithms, quantum search, quantum fourier transforms, quantum error correcting codes, quantum cryptography, nonlocality and quantum communication complexity, and quantum computational complexity.
PHYS677 Implementations of Quantum Information	B. C. Sanders	Proposals and realizations of quantum information tasks including quantum computation, quantum communication, and quantum cryptography in optical, atomic, molecular, and solid state systems.
PHYS673 Quantum and Nonlinear Optics	C. Simon	Theory of dispersion. Fast and slow light. Basics of nonlinear optics. Nonlinear optical crystals, phase matching. Coherence theory. Preparation, manipulation and measurement of quantum optical states and single-photon qubits. Elements of atomic physics, optical Bloch equation, rotating-wave approximation. Two-and three-level systems. Cavity quantum electrodynamics.



# SERVICES AND OUTREACH

## Conferences/Workshops

MEMBERS	COMMITTEE	CONFERENCE/WORKSHOP	LOCATION	DATES
P. Kennepohl	Inorganic Program Chair	2022 Canadian Chemistry Conference and Exhibition	Calgary, Canada	13–17 Jun 2022
P. Kennepohl	Organizer	2026 International Symposium on Halogen Bonding (IXSB)	Banff, Canada	2026
B. C. Sanders	Co-Chair	BIRS Workshop on New Development in Quantum Machine Learning	Banff, Canada	12–17 Jul 2020
B. C. Sanders	Chair, Program Committee	International Conference on Quantum Communication, Measurement and Computing	Lisbon, Portugal	11–15 Jul 2022

### **Professional Services**

NAME	ROLE	JOURNAL/SOCIETY/INSTITUTION
P. E. Barclay	Associate Editor	Optics Express
D. L. Feder	Member, Editorial Board	PLoS One
P. Kennepohl	Director, Reactive Intermediates Student Exchange Program	University of Calgary
P. Kennepohl	Chemistry & Catalysis Program Review Panel	Stanford Synchrotron Radiation Lightsource
P. G. Kusalik	Member, Advisory Board, US Department of Energy Frontier Research Centre "Fluid Interface Reactions, Structures and Transport (FIRST)"	Oakridge National Laboratory

NAME	ROLE	JOURNAL/SOCIETY/INSTITUTION
N. Moazzen- Ahmadi	Co-Editor, Special Issue	Journal of Molecular Spectroscopy
N. Moazzen- Ahmadi	Member, Editorial Board	Journal of Molecular Spectroscopy
D. R. Salahub	Member, Editorial Board	Advances in Quantum Chemistry
D. R. Salahub	College of Reviewers	Canadian Institutes of Health Research
D. R. Salahub	Member, Editorial Board	Computation
D. R. Salahub	Vice Chair, Editorial Board	Interdisciplinary Science: Computational Life Sciences
D. R. Salahub	Member, Editorial Board	Journal of Computational Chemistry
D. R. Salahub	Member, Academic Editorial Board	PLoS One
B. C. Sanders	Member, Editorial Board	IOP ebooks™
B. C. Sanders	Chair, Steering Committee	Quantum Africa Conference Series
B. C. Sanders	Editor-in-Chief	New Journal of Physics
B. C. Sanders	Member, SUPPORT Committee, VPR Catalyst Grants Program	University of Calgary
Y. J. Shi	Associate Editor	Canadian Journal of Chemistry
C. Simon	Member, Physics Advisory Committee	Fermi National Accelerator Laboratory (United States of America)
C. Simon	Members, NRC SDTech	National Research Council Canada
S. Trudel	Chair, Materials Division	Chemical Institute of Canada

### **Outreach Lectures**

8 July 2021, B. C. Sanders, "On quantum computing", CDL-Toronto Quantum Bootcamp (virtual). 4 February 2021, B. C. Sanders, "Quantum computing for data science", Synthetic Intelligence Forum (virtual), Toronto, Canada.

7 March 2021, D. Oblak, "Quantum information basics and teleportation", Rocky Mountain Junior Science Contest (virtual), Calgary, Canada.

## Media Coverage

SOURCE	TITLE OF ARTICLE	DATE
Physorg.com	Researchers discover new method to generate nanobubbles in water: Peter Kusalik	7 April 2020
Globe and Mail	Calgary man supplies 20,000 face masks to city's vulnerable populations: Chris Healey	29 April 2020
Calgary Herald	Mapping out Calgary's road to economic recovery: Quantum Computing	7 May 2020
Physorg.com	Scientists demonstrate quantum radar prototype: Shabir Barzanjeh	8 May 2020
UCalgary News	Faculty of Science researcher helps spearhead quantum radar prototype: Shabir Barzanjeh	11 May 2020
Times of India	RRI researchers' toolkit to aid secure communication: Barry C. Sanders	29 June 2020
Miragenews	CSIS warns about China's efforts to recruit Canadian scientists: Barry C. Sanders	6 August 2020
APS News	The quantum internet will require bigger quantum science (back page/volume 29/number 8): Christoph Simon	26 August 2020
Physicsworld.com	Molecule's electronic structure is simulated on a quantum computer: Barry C. Sanders	5 September 2020
University World News	Intelligence services warn against China's talents plan: Barry C. Sanders	12 September 2020
Science	The short weird life—and potential afterlife—of quantum radar: Shabir Barzanjeh	23 September 2020
University Affairs	The quest to build a reliable quantum computer: Barry C. Sanders	14 October 2020
UCalgary News	Formidable expertise in quantum computing earns postdoc award: A. Alase, B. C. Sanders and D. Feder	20 October 2020
Calgary Herald	Province gives \$11.8M to U of C for quantum research, other projects: Quantum Alberta & Quantum MIF Project	23 October 2020
UCalgary News	Class of 2020: Innovation and community define student experience for Governor General's Gold Medal winner: Matthew Mitchell	30 November 2020
UCalgary News	New study turns gold into magnets: Simon Trudel	3 December 2020
Chinadaily.com.cn	Quantum computer created: Barry C. Sanders	5 December 2020
Azoquantum.com	Scientists take important step toward building practical quantum internet: Daniel Oblak & Christoph Simon	16 December 2020

SOURCE	TITLE OF ARTICLE	DATE
Israel National	Fermilab and partners perform steady, high-fidelity quantum teleportation: University of Calgary	16 December 2020
UToday	Scientists take important step toward building practical quantum internet: Daniel Oblak & Christoph Simon	16 December 2020
Zive.cz	Quantum teleportation for 44 kilometers. The Americans put into operation the basic principle of the quantum Internet: University of Calgary	16 December 2020
Actu-cameroun.com	Weltnachrichten – AU – Researchers have achieved sustained long-distance quantum teleportation: University of Calgary	17 December 2020
Engadget.com	A successful experiment gets us one step closer to a quantum internet: University of Calgary	17 December 2020
Vice.com	Researchers have achieved sustained long-distance quantum teleportation: University of Calgary	17 December 2020
Yahoo News	A successful experiment gets us one step closer to a quantum internet: University of Calgary	17 December 2020
The Debrief	Quantum teleportation achieved, say team of leading scientists: Daniel Oblak & Christoph Simon	18 December 2020
Hypasos.com	Scientists discover quantum teleportation: University of Calgary	18 December 2020
Reccom	Quantum teleportation: research goes one step further: University of Calgary	18 December 2020
Sci Tech Daily	Sustained, high-fidelity quantum teleportation achieved for the first time: Daniel Oblak & Christoph Simon	18 December 2020
Independent.co.uk	NASA scientists achieve long-distance quantum teleportation that could pave way for quantum internet: University of Calgary	21 December 2020
Siliconrepublic	Researchers achieve long-distance quantum teleportation: University of Calgary	21 December 2020
UChicago News	Fermilab and partners achieve sustained, high-fidelity quantum teleportation: University of Calgary	28 December 2020
Sci-News	Researchers demonstrate high-fidelity quantum teleportation: University of Calgary	30 December 2020
UCalgary News	Top research stories of 2020: quantum physicists	5 January 2021
CBC Radio 1 (Calgary Eyeopener with David Gray & Angela Knight)	Quantum teleportation: Daniel Oblak	8 January 2021

SOURCE	TITLE OF ARTICLE	DATE
Radio Cananda	Scientists perform 44-kilometer quantum teleportation (French): University of Calgary	8 January 2021
Marshable	The dawn of the quantum internet (video): University of Calgary	20 January 2021
The Costa Rica News	did-nasa-achieve-long-distance-quantum-teleportation?: University of Calgary	30 January 2021
Livescience.com	Chinese researchers to send an 'uncrackable' quantum message to space: Daniel Oblak	1 February 2021
UCalgary News	University of Calgary's new nano-fabrication 'foundry' will advance quantum network devices: Paul Barclay	3 March 2021
Eureka Alert	The imaginary part of quantum mechanics really exists! : University of Calgary	25 March 2021
UCalgary News	Physics researchers achieve first-ever cooling of antimatter by laser: Rob I. Thompson & Timothy Friesen	31 March 2021



## RESEARCH GRANTS (UNAUDITED)

By origin



41

### By funding agency





# **OBJECTIVES FOR NEXT YEAR**

#### PAUL E. BARCLAY

- Report first demonstration of a universal optomechanical interface with quantum memory
- Demonstrate a diamond-superconducting cavity electromechanical devices
- Report cavity enhanced torque magnetometry at > 100 MHz

#### SHABIR BARZANJEH

- Measure optomechanical interaction in fridge
- Characterize electro-optomechanical samples for photon conversion

#### DAVID L. FEDER

- Extend the matrix-product formalism to higher bond dimension for qubit chains to find new resource states for measurementbased quantum computation
- Explore the relationships between graph states and topological error-correcting codes
- Probe the boundary between classically efficient and inefficient simulations of Boson Sampling

- Provide numerical and analytical support to experiments in the lab of Lindsay Leblanc to simulate non-Abelian operations in ultracold atomic gases
- Investigate possible exact solutions for the ground state of lattice hard-core bosons
- Complete analysis of two-component Bose-Einstein condensates in the presence of spin-orbit interactions and external rotation

#### TIM FRIESEN

- Commission ALPHA-g apparatus at CERN
- Install and calibrate Time Projection Chamber annihilation detector in the ALPHA-g apparatus
- Install and test new cylindrical Penning trap designs for antihydrogen formation and spectroscopy
- Trap and perform first gravitational free-fall experiments on antihydrogen in ALPHA-g apparatus

#### GILAD GOUR

• Determine necessary and sufficient conditions for converting one state to another under symmetric operations

2020-2021 ANNUAL REPORT

- Derive necessary and sufficient conditions for converting an incoherent athermal state to an athermal state with coherence in the energy basis
- Find an explicit example for non-additivity of the Holevo capacity of a quantum channel
- Generalize the uncertainty principle from a lone system to a system entangled with quantum memory with applications to quantum cryptography

#### PETER HØYER

- Prove a polynomially small error for a quantum walk
- Show electrical circuit bounds for quantum algorithms on graphs

#### PIERRE KENNEPOHL

- Synthesis and characterization of novel molecular spin qubits with long coherences times at "high temperature"
- Characterization of both halogen and chalcogen bonding motifs as mediators of electron communications
- Submit major grant proposal for laboratorybased x-ray spectroscopic and imaging instrumentation

#### PETER G. KUSALIK

- Examine the factors important in the stability and mechanism of formation of aqueous nanobubbles
- Develop and validate effective interaction potentials for hydroxide radical in water that faithfully reproduces the structural features observed from ab initio simulations
- Determine the stability and reactivity of hemi-bonded complexes of hydroxide radical with Cl- or Br- anions

- Develop and test empirical and coarse grain potential models appropriate for simulations studies of self-assembly processes in Zn/ carboxylate MOFs
- Use machine learning approaches to characterize formation of order during MOF self-assembly
- Develop Markov State models based on key structural events and their transitions during the nucleation processes of ice and gas clathrate hydrates
- Use novel molecular simulation approaches to identify nucleation and crystal growth pathways for potassium dihydrogen phosphate

#### NASSER MOAZZEN-AHMADI

- Design and test a photonic gas sensor for use at mid-infrared wavelengths
- Develop accurate global potential energy surfaces for molecular complexes
- Spectroscopically characterize microsolvation of carbon dioxide in rare gases

#### DANIEL OBLAK

- Demonstrate quantum communication with quantum satellite
- Create prototype system for measurementdevice independent quantum key distribution
- Show interaction of microwave field with rare-earth ion-doped material
- Detect and characterise spectrum of spontaneously emitted ultraweak photons from biological samples
- Spectroscopic studies of promising rareearth ion-doped materials for quantum memory and quantum transduction
- Show interface between photons emitted from quantum dots and rare-earth ion doped crystal

#### DENNIS R. SALAHUB

- Consolidate collaborative research with NRC-Ottawa within their Al4D (artificial intelligence for design) program on design of new nanocatalysts
- Explore rapid semi-empirical methods for strongly correlated system
- Extend DFT+U calculations to vacancies in Ni-ceria nanocatalysts
- Extend oil-sands upgrading simulations to molybdenum disulfide as the nanocatlyst; revisit MoC2 with machine-learning methods
- Consolidate the use of machine learning for global optimization problems; new functionality for deMon2k and QMLMaterials
- Explore the use of machine learning to identify reaction coordinates (collective variables) for free-energy calculations

#### BARRY C. SANDERS

- Complete a conceptual framework for interconnecting machine learning and control in both classical and quantum domains and apply this framework to significantly enhance quantum-gate fidelity in atomic quantum computing platforms
- Construct, employ and characterize quantum-enhanced computer programs for solving problems in energy and health sectors
- Develop a best-practice verification & validation framework for the quantum supply chain
- Deploy and test Calgary's quantum-satellite ground station (with Oblak)
- Complete theory on algorithmic quantum measurement as the dual to quantum state-generation algorithms
- Develop an enhanced quantum algorithm for quantum-field ground-state generation
- Complete proof that fermion sampling is hard if simultaneity is not guaranteed

#### CARLO MARIA SCANDOLO

- Identify states responsible for objectivity in general physical theories
- Determine how and when the behaviour of decoherences in general physical theories differs from the quantum one, and study its informational implications
- Use tools of resource theories beyond quantum information science, e.g. in dynamical systems
- Apply necessary and sufficient conditions for state conversion in dynamical resource theories to the case of quantum conditional majorization
- Formulate a second law of thermodynamics, with applications to quantum communication
- Achieve a mathematically rigorous treatment of PT-symmetric quantum mechanics

#### YUJUN SHI

- Further investigate chemical kinetics of nitrogen-containing organosilicon precursors in the chemical vapor deposition process
- Develop method for fabrication of semiconductor nanowires
- Explore the dewetting methods for formation of gold-containing bimetallic nanoparticles

45

#### CHRISTOPH SIMON

- Study the feasibility of quantum memories onboard satellites based on Bose-Einstein condensates, rare-earth ion-doped crystals, and hot vapours
- Develop theory of the fidelity of quantum transducers and quantum memories
- Create new types of photonic entanglement from quantum dot sources (with Senellart)
- Develop room-temperature quantum network architectures based on hot vapours and defects in two-dimensional materials
- Develop cavity-enhanced and on-demand quantum memories
- Develop quantum information processing applications of Rydberg excitons (with Heshami)
- Explore potential instances of the radical pair mechanism in neuroscience
- Detect and characterize biophotons emitted by neurons (with Oblak and McFarlane)
- Explore the potential role of biophotons in learning in the brain (with Nicola)

#### **ROB I. THOMPSON**

- Commission ALPHA-g apparatus at CERN to collect antimatter gravity data during fall 2021 antiproton beam time
- Resolve atomic structures of antihydrogen
- Develop laser-based ion-source options for TITAN

#### SIMON TRUDEL

- Investigate polyamorphous behaviour in metal oxides
- Develop solution-processable solar cells
- Study mechanism of small-molecule transformation with metal-oxide electrocatalysts

#### **ROBERT A. WOLKOW**

- Explore quantum sensing and metrology with the new atom-scale fabrication-andinspection tool at a temperature of one Kelvin and magnetic field of five Tesla
- Prepare a new lithographic tool for operation
- Combine quantum characterization techniques with atomic patterning and characterization to evaluate spin character of electron- and hole-based quantum dots (with Ladrière)
- Begin design, fabrication and testing of an atom-defined quantum comparator device with Texas Instruments and Quantum Silicon
- Develop the transmission line impedance matching chip layout to enable classical applications and quantum characterisation
- Update "SiQAD", a computer aided design tool for layout and modeling of atomic circuitry created with Professor Konrad (with Walus) including a capacity to treat atom-defined metal circuit elements within a finite-element electrostatic modeling approach
- Model geometric and electronic structure and electrical transport properties of silicondangling-bond-based atomic structures, e.g. single and double quantum dots, nanowires (with Guo and Smeu)
- Develop quantum metrology devices to serve as current and temperature standards (with Todd, Sanchez and Pitters)
- Measure with scanned multi-probe techniques the electronic and geometric structure of silicon atomic wires

# IQST ADDS VALUE TO THE UNIVERSITY OF CALGARY IN THE FOLLOWING WAYS

Enables multidisciplinary research through financial and logistical support

Builds a quantum science and technology community through visitor, seminar, and colloquium programs

Assists new faculty members to becoming productive researchers rapidly

Publishes reports and web pages that showcase the Institute as a leader in quantum information science

Supports recruitment of outstanding faculty, researchers, and graduate students

Sponsors and supports leading conferences held locally

Partners with other quantum institutes

Enhances the University's reputation by delivering outstanding research results

Benefits the wider community by contributing new knowledge in a strategic area

### IQST.CA @iqstucalgary

Phone: (403) 220-4403 Fax: (403) 210-8876 Email: iqstinfo@ucalgary.ca

INSTITUTE FOR QUANTUM SCIENCE & TECHNOLOGY University of Calgary 2500 University Drive NW Calgary, AB T2N 1N4 Canada