

2020 News Items

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Peer-reviewed Publication for Chemistry Faculty Member, Dr. Cory C. Pye

December 4, 2020

An ab initio investigation of the second hydration shell of metal cations, Computers and Applied <u>Chemistry</u>, published in the journal "Computer and Applied Chemistry"; Authors: **Cory C. Pye** and Courtney R. Gilbert (née Schaller)

Co-author Courtney Gilbert is a graduate of Saint Mary's University.

SMU Chemistry Faculty Members, Christa Brosseau and Clarissa Sit, collaborate to make new pet wellness products.

November 23, 2020

When Baie Run Pet Products, a health and wellness pet company focused on dogs and cats' wellbeing, wanted to improve their pet supplements, they turned to Saint Mary's experts for advice. The company worked with Dr. Christa Brosseau and Dr. Clarissa Sit to develop a manufacturing process for colloidal silver that the manufacturer could follow. You can read how Drs. Brosseau & Sit's assisted with Baie Run's new formulation <u>here</u>

Chemistry Student, Kaleigh McLeod, part of a group of Undergraduate Students spending their summer conducting paid scientific research

October 2, 2020

Kaleigh McLeod, under the supervision of <u>Dr. Christa Brosseau</u>, received her award, as part of a group of <u>Science Undergraduate Students conducting scientific research</u>. The awards are sponsored by the Natural Sciences and Engineering Research Council (NSERC), a Government of Canada agency, and the Dean of Science Office at Saint Mary's University. These awards are intended to help students develop their potential for a research career in the natural sciences and engineering, and often lead to students pursuing graduate work in their chosen fields.

Kaleigh received her award on her research project in how to make an all wood-pulp N95 respirator as part of our COVID-19 project with Port Hawkesbury Paper. She is continuing the project on for the rest of this academic year as her honours project in Chemistry. To read more about her, other Undergraduate Students, and their research projects, <u>visit</u>.

Congrats Kaleigh!





Chemistry Faculty Member, Dr. Jason Masuda, receives NSERC Funding.

September 18, 2020

Dr. Jason Masuda, as a part of a group of <u>Saint Mary's Scientists awarded \$1.6 Million in NSERC</u> <u>Funding</u> for his **Stabilization of Unique Chemical Bonding Environments and Exploration of Small Molecule Reactivity** research.

Work in the research group, lead by Dr. Masuda, is focussed on the preparation of new functional groups specific groups. Functional groups are arrangements of atoms within molecules that have characteristic properties, such as aldehydes, ketones, and alcohols. Chemists have a general understanding of how normal functional groups react. In the Masuda group, new arrangements of atoms are targeted and once isolated, the physical properties are studied as well as how they react with other molecules.

Most importantly, student researchers in the Masuda Group learn transferrable skills, such as critical thinking and organizational skills, that will assist them as they move on in their careers.

Congrats Jason!

SMU Chemistry Students and Faculty help create rapid test kit for COVID-19

July 23, 2020

When students and faculty at Saint Mary's were starting the winter 2020 term in January, the plan was for a normal busy university term of classes and labs. Two months later students, faculty and staff were adjusting to the new normal of working and studying from home during a quickly-evolving global pandemic, and the world looked very different by April. That same month, a a quickly formed small team of Chemistry researchers, including undergraduate students, started working on a vital contribution for a rapid, point-of-care, Covid-19 test kit, created by a startup company in Dartmouth, NS. For more on this collaboration, visit.

Peer-reviewed Publication for Chemistry Faculty Member, Dr. Cory C. Pye.

July 13, 2020

Desymmetrization in geometry optimization: application to an ab initio study of copper(I) hydration, Published in the journal "Pure and Applied Chemistry", vol. 92, iss. 10; Authors: **Cory C. Pye**, Daniel C. M. Whynot, Christopher R. Corbeil, Darren J. W. Mercer

Co-authors Whynot, Corbeil and Mercer are former graduates of Saint Mary's University

Peer-reviewed Publication for Chemistry Faculty Member, Dr. Jason D. Masuda.

July 15, 2020

Synthesis and structural characterization of methylindium imino/aminophenolates: Comparison to aluminum analogues and reactivity toward the coupling reactions of carbon dioxide with epoxidesm, Published in the "Journal of Organometallic Chemistry", vol. 919; Authors: Kori A. Andrea, Adam R. Beckett, Glen G. Briand, Sarah A. Martell, **Jason Masuda**, Kathleen M. Morrison, M.T. Emilie Yammine.





Peer-reviewed Publication for Chemistry Faculty Member, Dr. Cory C. Pye.

June 10, 2020

<u>Chemical Safety: TATP Formation in 2-Propanol</u>, Printed in the American Chemical Society's publication "Chemical Health and Safety"; author: **Cory C. Pye**

Chemistry Faculty Member, Christa Brosseau, exploring way to produce medical grade N95 respirators using wood pulp

May 12, 2020

Dr. Brosseau and her research team are in collaboration with the pulp and paper industry in Nova Scotia, developing and testing chemical additives that can address key challenges in the production of medical-grade pulp from thermomechanical pulp for the use of manufacturing N95 masks. To learn more about her research, <u>visit</u>

Peer-reviewed Publication for Chemistry Faculty Member, Dr. Jason D. Masuda.

May 5, 2020

A Rare Low-Spin Co(IV) Bis(β-silyldiamide) with High Thermal Stability: Steric Enforcement of a <u>Doublet Configuration</u>, Published in the journal "Angewandte Chemie International Edition", vol. 59, iss. 33; Authors: David Zanders, Goran Bačić, Dominique Leckie, Damilola O. Odegbesan, Jeremy Rawson, **Jason D. Masuda**, Anjana Devi, Seán T. Barry

Peer-reviewed Publication for Clyburne Research Group

April 16, 2020

Heavy metals make a chain: a catenated bismuth compound, Published in "Chemistry: A European Journal", vol. 26, iss. 34; Authors: **Robert D. Riley**, Diane A. Dickie, **Michael A. Land**, Richard A. Kemp, Charles L. B. Macdonald, Ulrike Werner-Zwanziger, **Katherine N. Robertson**, **Jason A. C. Clyburne**

Congrats to the Clyburne group! Robert is a SMU Chemistry Honours graduate and Micheal graduated from SMU with both a BSc(Honours) and an MSc. This project involved collaborators from Dalhousie University, Carleton University, and the University of New Mexico.

Peer-reviewed publication for Chemistry Faculty Member, Dr. Cory C. Pye

April 15, 2020

An ab initio study of the effect of hydration on the vibrational spectrum of hydrogen sulfate, Published in the journal "Computational and Theoretical Chemistry", vol. 1176; Author: Cory C. Pye

This paper uses ab initio theory to interpret the differences in the Raman spectra of the hydrogen sulfate ion (HSO4⁻) in gas-phase, aqueous solution, and the counterion in hexylmethylimidazolium hydrogen sulfate ionic liquid.





SMU Chemistry Students and Faculty members help with hand sanitizer project

April 14, 2020

With the scope of the global COVID-19 pandemic expanding quickly, Honours Chemistry students Julie Dayrit and Prashansa Kooshna wanted to help, hoping that they might be able to produce hand sanitizer in now-vacant chemistry labs after the closure of the Saint Mary's University campus. More about their project may be found <u>here</u>.

Chemistry Student, Jennifer Kolwich, awarded first prize in writing competiion

April 2020

Jennifer Kolwich was awarded a First Prize in the Post Graduate Category for her paper "*Fighting Fungus with Fungus: A Microbe-Based Solution to Bat White-nose Syndrome"*, a Student Science Writing Competion hosted by the <u>Nova Scotian Institute of Science (NSIS</u>).

Congrats Jenn!

Peer-reviewed Publication for Chemistry Faculty Member, Dr. Cory C. Pye

March 21, 2020

<u>One-Dimensional Cluster Analysis and its Application to Chemistry</u>, Published in the journal "The Chemical Educator", vol. 25; Author: **Cory C. Pye**

This paper rigorously defines the idea of clustering in data and illustrates its use to help assign the 1H-NMR spectrum of ethyl acetate, the gas-phase infrared spectrum of carbon dioxide, and the microwave spectra of the alkali halides CsI, CsBr, RbI, RbBr, and KI.

This paper is dedicated to Professor Emeritus John C. O'C. Young on the occasion of his 90th birthday.

Chemistry Research Associate, Dr. Kathy Robertson, recipient of award.

March 6, 2020

Dr. Kathy Robertson is the 2020 recipient of the Saint Mary's University Faculty of Graduate Studies and Research Staff Research Recognition Award. Dr. Robertson is an integral part of the Clyburne research group and also plays an important role in the department as the local crystallography guru and collaborator. Since starting at SMU in 2010, she has amassed over 40 peer-reviewed publications.

Congrats Kathy!

Chemistry Faculty Member, Dr. Cory C. Pye, recipient of research grant

March 2020

Cory Pye is a co-investigator on a successful Compute Canada Research Platforms and Portals proposal of Raymond Poirier (MUN) entitled "Retrievium: The element of discovery". The aim is to develop a computational chemistry platform for storage retrieval, and mining of computational chemical data.





Peer-reviewed publication for Sit Research Group

March 2020

Does size matter? An investigation into the impact of coarse and fine ground inoculated biochar on Hordeum vulgare (barley) growth and yield, Published in the journal "Rhizosphere" Vol. 17; Authors: Kaitlyn L. Blatt-Janmaat, Stephanie L. MacQuarrie, Clarissa S.Sit

This is the first publicaiton from the Sit Research Group in 2020. Researcher Kaitlyn Blatt-Janmaat is a recent SMU Chemistry Honours (and biology major) graduate.

Peer-reviewed publication for Chemistry Faculty Member, Dr. Cory C. Pye

February 25, 2020

An Ab Initio Investigation of the Hydration of Thallium(III) and Mercury(II), Published in the "Journal of Solution Chemistry", vol. 49; Authors: **Cory C. Pye** and C. Mahesh Gunasekara

This paper uses ab initio theory to benchmark several effective core potentials for hydrated mercury(II) and thallium(III) aqua ions, focusing on the incremental hydration energies, bond lengths, and totally symmetric M-O vibrational frequency

Peer-reviewed publication for Chemistry Faculty Member, Dr. Jason A. C. Clyburne

February 19, 2020

<u>Canadian bitumen is engineered for transport, but the type of product produced can affect spill</u> <u>contingency planning</u>, Published in the journal "Environmental Science: Processes & Impacts", iss. 4; Authors: Thomas L. King, Brian Robinson, Scott Ryan and **Jason A. C. Clyburne**

Dr. Thomas King is a recent graduate from the Saint Mary's PhD program in Applied Sciences.

Fourth Year Chemistry Student, Maddison Eisnor, wins national award

February 18, 2020

Maddison has won the <u>Chemical Institute of Canada's CIC Analytical Chemistry Division</u> <u>Undergraduate Travel Award</u> in Honor of Dr. Nick Toltl. The award will allow Maddison the opportunity to talk about her 2D-LC (Two-Dimensional Liquid Chromatography) research on polyphenols at the 103rd <u>Canadian Chemistry Conference and Exhibition</u> in Winnipeg, Manitoba. To learn more about her national award, <u>read here</u>.

Congrats Maddy!

Peer-reviewed publication for Chemistry Faculty Member, Dr. Jason D. Masuda

January 21, 2020

Volatile and Thermally Stable Polymeric Tin Trifluoroacetates. Published in the American Chemical Society's "Inorganic Chemistry" edition, vol. 59, issue 2; Authors: Bačić, G., Rankine, C.D.; Masuda, J.D.; Wann, D.A.; Barry, S.T





Peer-reviewed publication for Brosseau Research Group

January 10, 2020

Spectroelectrochemical and computational studies of tetrahydrocannabinol (THC) and carboxytetrahydrocannabinol (THC-COOH), Published in the journal "Analyst", issue 5; Authors: Shruti D. Bindesri, Ricardo Jebailey, Najwan Albarghouthi, Cory C. Pye, Christa L. Brosseau

This is the first publication from the Brosseau group in 2020. Representing the group are: Shruti (a Chemistry Honours student), Ricardo (a SMU undergraduate student), Najwan (a SMU PhD student) and Dr. Christa Brosseau. SMU Chemistry faculty member, Dr. Cory Pye provided support in the collaboration by providing ab initio calculations.

Peer-reviewed publication for Chemistry Faculty Member, Dr. Jason Masuda

January 9, 2020

A one-pot method for the synthesis of 3-(hetero-)aryl-1,4,2-dioxazol-5-ones, Published in the "Canadian Journal of Chemistry", vol. 8, no. 93; Authors: T. Hynes, D.S. Hall, A.W.H. Speed, J.D. Masuda, J.R. Dahn

