

Q-CHeM CHRONICLES



Dr. Jessop (right), receiving the Eni Award from the President of Italy (Mr. Giorgio Napolitano, centre) and the President of Eni Corp. (Mr. Giuseppe Recchi, left).

A Banner Year for Dr. Jessop and His Research Group

It's been an exciting year for Dr. Philip Jessop and his group! Last summer, Dr. Jessop was awarded the Eni Award for New Frontiers for Hydrocarbons (Upstream), including a gold medal from the President of Italy, awarded at the presidential palace in Rome. Eni, a European oil company, created these prestigious awards many years ago to recognize academic research on needs in the energy industry. The event included a private tour of the Vatican Museum and Sistine Chapel, and a banquet in the

Vatican gardens. During the past year, Dr. Jessop also received a Tier 1 Canada Research Chair, announced in March 2014, and was elected a Fellow of the Royal Society of Canada, which became official in a ceremony in Banff in November 2013.

Dr. Jessop was on a year-long sabbatical from July 2013 to June 2014 and, during that time, he was the Landolt & Cie Professor in Innovations for a Sustainable Future, an invited chair position at the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland. He also

travelled extensively, giving invited lectures at universities and conferences in Spain, France, UK, Germany, Switzerland, Sweden, Italy, Hungary, and Singapore. This allowed him to establish new collaborations with scientists at EPFL and across Western Europe.

Recognition has come to students in the group as well. Current MSc student Jeremy Durelle received the Christopher Knapper Award for Excellence in Teaching Assistance. The work of recent MSc graduate Elize Ceschia, who discovered that switchable surfactants could clean up oil spills and recover the oil, was covered as a news story in *Chemistry World*. The work of Jesse Vanderveen and Jeremy Durelle on developing switchable-hydrophilicity solvents was highlighted in *Chemical Views* magazine. PhD students Vanessa Little and Trisha Ang successfully defended their dissertations.

The Jessop group members now hold six issued patents on switchable solvents and switchable surfactants. Mathematical models and physical chemistry data on the solvent behaviour are being combined with predictions of environmental and health impact, in a chemical informatics approach, to design the greenest switchable solvent possible. Forward Water Technologies Inc., the second spinoff company based upon a Jessop technology, was created to commercialize a switchable osmosis method for purifying seawater or wastewater. Research in CO₂-related solvents has included extraction of bio-oil from algae and valuable phenolic compounds from lignin pyrolysis oil (from sawdust or tree bark).

The Jessop group has been collaborating with Dr. Michael Cunningham (Chemical Engineering) on developing switchable materials, including polymer latexes that can be coagulated and then resuspended; the conversion of bulk solid polymers into latexes; the creation of solid surfaces having switchable

properties; and the design of switchable polymers for forward osmosis purification of wastewater. With Dr. Guojun Liu, the group has made switchable drying agents (solids that will capture water out of organic liquids). CO₂ chemistry is a major emphasis in the Jessop group, and not just for making things switchable. Current projects include uncatalyzed reactions of CO₂ and CS₂ with amidines; the design of new catalysts, using abundant rather than precious metals, for the hydrogenation of waste CO₂ into useful organic chemicals; and catalytic methods, either with or without CO₂, for the asymmetric hydrogenation of C=C bonds that are far from other functional groups.

GreenCentre Canada, where Dr. Jessop serves as technical director, has had its federal funding renewed for another five years. In 2013, the centre received its 500th technology disclosure, hosted its second Sustainable Chemistry Summit, created a third spinoff company, and awarded \$791,000 to small and medium businesses for development of new green chemistry technologies. Dr. Jessop also serves on the editorial board of the journal *Green Chemistry*, the governing board of the American Chemical Society's Green Chemistry Institute, and the NSERC Discovery Grants panel for the evaluation of chemistry-related proposals. With Dr. Cunningham, he co-edited a special issue of the journal *Green Materials*, dedicated to CO₂-triggered switchable materials. Finally, Dr. Jessop will be the lead organizer of the environmental division programming for the 2015 Canadian Chemistry Conference, hoping to encourage the next generation of green chemistry research and technologies.

While the past year has been full of excitement, Dr. Jessop and his group continue looking towards the future, to discoveries of new technologies that take advantage of the properties and abundance of waste carbon dioxide.

2013-2014 Departmental Highlights

JUNE 2013

- Jean-Michel Nunzi and co-applicants Drs. J. Stotz from Physics and D. Bartz from Chemical Engineering are awarded a \$400,000 grant by the CFI Leaders Opportunity Fund, for their project "Research on Portable Multidimensional Micro-Nano Biological Sensing Devices."
- Tucker Carrington is chosen as the winner of the 2013 Gerhard Herzberg Award given by the Canadian Society for Analytical Sciences and Spectroscopy.
- Robert Gordon, a Chemistry Professor Emeritus, receives the 2013 Capital Distinguished Citizen Award from the Mayor of Kingston for his committed volunteerism in the community.
- Thomas Kraft (Nunzi group) is awarded a scholarship by the Embassy of France in Ottawa for his research on Carbon Nanotube Solar Cells.

JULY 2013

- Eric Keske (Crudden group) is selected for the Dobbin Scholarship on behalf of the board of the Ireland Canada University Foundation.

SEPTEMBER 2013

- Brian Bestvater (Crudden group) is the recipient of the 1960's Chemistry Scholarship, which was established by members of the chemistry classes from the 1960s to acknowledge the outstanding education they received in the Chemistry Department.
- Xiang Wang (Wang group) receives the McAdie Doctoral Student Award.
- Gabriele Schatte joins the department as our Instrumentation Manager in the X-Ray Diffraction and Surface Analysis Facilities.

OCTOBER 2013

- Gregory Jerkiewicz is appointed to the Advisory Board of FC Cubic (Japan), the Fuel Cell Cutting-Edge Center Technology Research Association.
- The Queen's Chemistry Innovation Council Annual Meeting is held on October 17. The QCIC Welcoming Dinner speaker is Dr. Ted Hsu, a Queen's alumnus and Member of Parliament for Kingston and the Islands.
- PARTEQ Innovations signs a commercial agreement with Tianin Jet-Mate Technologies, a China-based company, for luminescent materials developed by Suning Wang's group.

NOVEMBER 2013

- Jason Vlahakis joins the department as a Laboratory and Student Training Coordinator.
- Jean-Michel Nunzi is renewed as a Tier 1 Canada Research Chair in Photonics for Life.
- Philip Jessop is elected to be a Fellow of the Royal Society of Canada and is the Landolt & Cie Professor in Innovations for a Sustainable Future at the École Polytechnique Fédérale de Lausanne in Switzerland for the 2013-2014 academic year.

DECEMBER 2013

- The annual holiday lunch is held Friday December 20, in the 4th floor lounge.
- Guojun Liu is awarded \$364,000 from the NSERC CRD program to develop an oil and water repellant industrial coating in collaboration with Lorama.

Message from the Head



Change is in the air! Last year at this time, the department was in the midst of a faculty search as part of the relaunched Queen's National Scholar (QNS) program. We are happy to announce that Dr. Avena Ross will be joining the department in January 2015 as a QNS in Chemical Biology. A brief bio of Dr. Ross can be found on page 10 of the Chronicles.

We welcomed Dr. Gabriele Schatte and Dr. Jason Vlahakis to the department in 2013. Dr. Schatte has taken the helm in our X-ray and Surface Analysis Facilities, bringing her many years of experience with research instrumentation, most recently at the Saskatchewan Structural Sciences Centre, to Queen's. Dr. Vlahakis will be familiar to many – he has a BSc and PhD from Queen's and, most recently, has been a postdoctoral researcher with Dr. Walter Szarek. Dr. Vlahakis brings a broad knowledge of chemical synthesis to our undergraduate program, as our Laboratory and Student Training Coordinator.

Our first year course, CHEM 112, has changed: We transitioned to a blended format that combines lectures, weekly

tutorials and labs, assigned readings, and online resources and homework. Organization and coordination were essential to the successful launch and we thank Nick Mosey for tackling the inevitable, unexpected hiccups that follow such a large change in format, and Michael Mombourquette and Len Rose for keeping the labs humming along, despite a new suite of experiments. There was an addition to the graduate course offerings this past year: The inaugural offering of CHEM 894-Business Skills in the Chemical Industry was a big success! QCIC members, Drs. Will Rogers and Wayne Schnarr led the initiative with a series of lectures presented in the fall. The course culminated with a day of graduate student presentations that focused upon potential commercialization of discoveries by Queen's chemists.

This year, 35 students graduated with Chemistry BSc degrees and 19 students graduated with degrees in Engineering Chemistry. Mei-Ni Belzile was both the Departmental Medal recipient, given to the graduating student with the highest GPA, and the recipient of the Smith Prize, given in recognition of excellence in undergraduate research by an Honours Chemistry student. The 2014 Society of Chemical Industry Merit Award was awarded to Jason Rygus and the Sullivan Prize was awarded to Xin Zhang for research excellence by a graduating Engineering Chemist.

This year's QChem Chronicles cover article spotlights Dr. Philip Jessop and his research group. They've had a busy and productive year, marked by discoveries, accomplishments and awards. Most notably, Dr. Jessop is the 2013 recipient of the prestigious Eni Award for New Frontiers of Hydrocarbons-Upstream. Highlights from the year are also included in this issue of the Chronicles, with details

on the new Chemistry website, on the newly-launched Harrison/MacRae Family Lecture Series, on recent research led by the Crudden and Horton groups, on the upcoming celebration in honor of Prof. Ken Russell's 60 years at

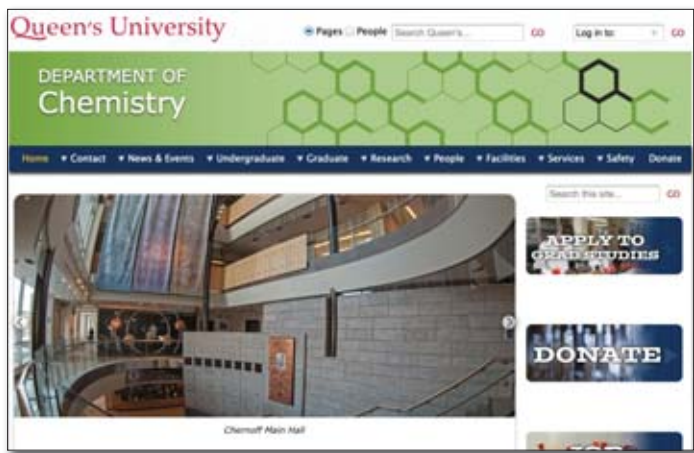
Queen's, and on brief profiles of award-winning faculty and students. Finally, Anne Petitjean and Michael Mombourquette reflect on the many contributions of Professors Henryka Tilk and Bill Newstead, as they both retire July 1, 2014.

New Website Launch

By Igor Kozin

In the digital world we all live in, it is essential that the various resources and services offered by the Department of Chemistry are accessible online. The departmental website is a valuable source of information to current and future students, researchers and collaborators, alumni and friends, and administrative staff.

In 2013, the departmental IT subcommittee was charged with a difficult task: design a new Chemistry website that incorporates such features as intuitive browsing, easy access to information, compatibility with different browsing platforms and mobile devices, and great visual appeal and functionality. Technical expertise for this project was provided by the Queen's School of Graduate Studies, and we are especially grateful to Colette Steer and her team for the enormous help they provided with the initial configuration, design and formatting of new webpages. The website project has also been supported by Queen's IT services and Marketing, and we thank Greg Black for the fancy photos and Lindsey Fair for marketing advice.



Our website will be hosted on Queen's servers, which brings numerous added benefits, including web security, uninterrupted technical support, and future software updates provided by Queen's IT personnel.

Website development and updating is a never-ending process but we are happy to report that, thanks to the hard work of the IT subcommittee members and departmental staff, especially Ed Maracle, Barb Armstrong, Michelle Boutilier, Meredith Richards and Annette Keyes, the new website is expected to be launched in July 2014. We hope that everyone will appreciate the website functionality, and the clean and attractive-looking interface. Bear in mind though that improvements and information updates will keep coming!

Business Skills in the Chemical Industry (CHEM 894), a New QCIC-led Initiative

By Will Rogers and Wayne Schnarr

The inaugural offering of CHEM 894 was a resounding success!

CHEM 894 is a graduate course designed to provide an overview of the business skills critical for success of the technical professional in the chemical industry. Developed by QCIC members Will Rogers and Wayne Schnarr, with the able assistance of 4th year Queen's Commerce student Wenhan Chen, the course featured four 3-hour lectures on:

- R&D Project Management – Planning for Innovation;
- Marketing & Business Strategy – Finding the Competitive Advantage;
- Organizational Design & Managing Systems – Executing Flawlessly;
- Financial Accounting & Analysis.

While the lectures covered some basic business knowledge, the ability to apply this knowledge as part of a team was developed during projects on technology commercialization that were

based upon research being carried out within the Queen's Chemistry Department. The teams recommended commercialization plans based on technology assessment, business analysis, and market and intellectual property strategies. The students presented their team's recommendations to their peers and the professors whose project the work was based upon.

Overall 15 graduate students took the course for credit, while several others audited. Feedback on the inaugural offering was strong and excellent suggestions for improvement were offered. Graduate student Tamara de Winter noted that "The course was the best experience that I have obtained at Queen's. Having Chemistry Alumni in the business world teach this course was an amazing opportunity." At the same time, Kyle Bachus noted "I was able to gain knowledge of how the business-side of chemistry operates.... It was during this final project that I



2013-2014 Departmental Highlights

learned the importance of the skills I had learned in lecture, teamwork, communication, and how to bring these together to accomplish a complete business analysis... I would recommend this course to any graduate student”.

The final project presentations proved to be outstanding. Will Rogers commented “I was absolutely impressed with the quality of the recommendations, the depth of the analysis and capability of the students to present and write-up their work.” The four projects were:

- Market Potential of a Novel Superamphiphobic Polymer Coating (Guojun Liu)
- Technology Assessment N-heterocyclic Carbene Self-assembled Monolayers (SAMs) on Gold (Cathleen Crudden and Hugh Horton)
- Business Evaluation of (-)- α -Kainic Acid (Andy Evans and Phillip Inglesby, Liverpool)
- Avisense Technologies – vibration sensing technology based on a fibre optic sensor (Peter Look)

Commenting on the presentation, Cathy Crudden noted that the work on SAMs was “truly exceptional and provided a valuable overview of the market opportunity”. Echoing Cathy’s comments Andy Evans noted “It is really rewarding that the students not only saw the commercial potential of kainic acid, but they also identified the same potential problems”.

“I was really pleased with how CHEM 894 was received by our students and faculty. Feedback on the course was very strong and we will definitely offer the course next year.” said Natalie Cann, Head of the Chemistry Department. Finally Wayne Schnarr commented “CHEM 894 is a great example of how QCIC can provide expertise and value to the department.”

JANUARY 2014

- Simon Hesp is interviewed by the Toronto Star on his research collaborations with MTO and the City of Kingston to build roads with a significantly reduced life-cycle cost. The article was followed by TV interviews with CBC Ottawa, CKWS and Global News Toronto.
- Bill Newstead is the recipient of the Engineering and Applied Science 1st year Instructor Award, this is Bill’s 8th time winning the award.
- Philip Jessop is the recipient of a \$378,240 Strategic Grant from NSERC and is a co-recipient of two more Strategic Grants (headed by Pascale Champagne and Michael Cunningham) totaling another \$945,330.
- Tucker Carrington receives the 2014 J.C. Polanyi Award in recognition of research excellence in physical chemistry, chemical physics, theoretical chemistry, or computational chemistry.

FEBRUARY 2014

- Julia van Drunen (Jerkiewicz group) is awarded a FAPESP Postdoctoral Fellowship to pursue research at the Universidade de São Paulo in Brazil.
- Victor Snieckus is honored by colleagues and friends with the publication of two dedicated volumes in the January 2014 issue of *Heterocycles*, in honor of his contributions to synthetic organic chemistry, especially to the Directed *ortho* Metalation (DOM) reaction which has received wide application in the preparation of pharmaceuticals (anti-AIDS, anti-inflammatory) and agrochemicals (antifungal for grain crops).

2013-2014 Departmental Highlights

MARCH 2014

- The Undergraduate DSC banquet is held on March 22. Nicholas Mosey receives the Faculty of the Year Award, Mark Raycroft (Stan Brown group) receives the TA of the Year Award, and Francoise Sauriol receives the Staff of the Year Award.
- Philip Jessop is awarded a Tier 1 Canada Research Chair in Green Chemistry.
- Bill Newstead is the Queen's University recipient of the Ontario Undergraduate Student Alliance Teaching Award.

APRIL 2014

- Zachary Hudson, former PhD student in the Wang group, is appointed Assistant Professor at the University of British Columbia.
- A publication by Department of Chemistry researchers, Cathy Crudden, Hugh Horton, Gang Wu and Nick Mosey is highlighted by Chemistry World (RSC). The publication describes to use of carbon-based ligands on gold in place of the more commonly employed thiols.
- Cathy Crudden is awarded a CIC Fellowship through the Chemical Institute of Canada.
- The 4th year project presentations are held on April 7. The Smith Prize is awarded to Mei-Ni Belzile and the Sullivan Prize to Xin Zhang. Ken Stevens and Will Rogers, members of the QCIC, judge both competitions and present the awards.

- The following students win national NSERC awards for 2014-2015: Joshua Clarke (Crudden), Molly Dushnicky (Evans), Soren Mellerup (Wang), Jason Rygus (Crudden), Caitlin Miron (Petitjean), and Jacqueline Seguin (Stan Brown and Zechel).
- Ontario Graduate Scholarship recipients for 2014-2015 are: Amy MacLean (Loock), Jesse Vanderveen (Jessop), Tamara DeWinter (Jessop), Michael MacLean (Crudden), Gurpaul Kochhar (Mosey), and Gillian Mackey (Stephen Brown).

MAY 2014

- Following the celebration of Alfred Bader's 90th birthday at Queen's, C&EN News (April 28 issue) published a laudatio article citing Victor Snieckus: "Alfred Bader's name is synonymous with helping chemists to make molecules; furthermore, his support through awards, fellowships, and scholarships is unwavering. But more than that, Alfred, with Isabel at his side, has touched all whom he has met with enthusiasm about their work and a zest for life."
- Diane Beauchemin's research on a new forensic tool to determine a person's gender and ethnicity through a thread of hair is featured in Chemistry World.

A Spotlight on Professor Henryka Tilk

by Anne Petitjean

Dr. Henryka Slebocka-Tilk is retiring this summer... Although this has been in the works for a couple of years, it is still hard for students and faculty to imagine the department without her constant and strong involvement in their everyday life.

After solid training at the Technical University (BSc) and Polish Academy of Science (PhD in radiation chemistry), Dr. Tilk pursued research in mechanistic chemistry in Texas (Dr. Kice), Toronto (Dr. Tidwell) and Edmonton (Dr. Brown). Luckily for us, when Dr. Stan Brown moved to Kingston in 1995, he convinced Henryka to move as well. While keeping up with research in the Brown lab, she initiated the position of Organic Lab Coordinator and built a consistent ensemble of experiments for all the organic chemistry courses in the undergraduate program, refreshing, complementing and enhancing the experimental training of our young students with one emphasis: showing how chemistry is engrained and relevant in our lives.

Student surveys show the excitement and interest these organic labs have generated. At the same time, teaching assistants in charge of training undergraduates in experimental chemistry have benefitted greatly from Dr. Tilk's unfailing supervision and high standards. Surely, their training in the highest safety standards, precise experimental procedures and professionalism will serve them well for the rest of their lives.



They will certainly fondly remember pizza breaks on days when exams had to be marked!

Dr. Tilk's commitment to the department has extended well beyond the organic chemistry labs. She taught Organic Chemistry for the Life Sciences for over a decade, with more than 7000 keen students having attended and dissected her lectures, an endurance that few instructors display. It isn't a surprise that Dr. Tilk cannot walk incognito in Kingston anymore! "Orgo" may not be the pre-meds' favourite topic at the start of the term, but many warmed up to it with Dr. Tilk's teaching. Her well-prepared lectures were reassuring and informative, but most importantly the relevance of chemistry was evident. From lessons in history to discussions of steroids, Dr. Tilk guided the students into real life chemistry. And who could better talk about organic transformations that changed our view of chemical reactivity than someone who had run that research first hand? What a treat to be taught the addition of bromine

to olefins and the discovery of the bromonium ion by the first author of the seminal JACS paper (1985, with Dr. Stan Brown) which reported the structure of this unusual intermediate! Through relevant examples, subtle jokes and great care for the students, Dr. Tilk has accompanied thousands of pre-meds through the demanding path of Orgo, with great effort and selflessness, volunteering her

Saturday mornings for special sessions.

With a passion for Chemistry, Dr. Tilk is not without other interests. Travel, music and visual art will keep her busy in the coming years, and you may find her attending a few Queen's Fine Art or Film Studies courses, as she's been known to do sometimes, sneaking into the lecture theater after her own classes! See you around, Dr. Tilk!

Dr. Avena Ross Joins the Department as a Queen's National Scholar

In 2012/2013, Queen's relaunched the university-wide Queen's National Scholar (QNS) program with a competition for two faculty positions. The Chemistry Department's nomination of Dr. Ross, as a QNS in Chemical Biology, was successful in the competition. In conjunction with Dr. Ross's arrival, the development of a new Honours program in Chemical Biology is underway, in collaboration with the Department of Biomedical and Molecular Sciences.

Dr. Ross was born in Manitoba but grew up in New Zealand where she attended the University of Auckland. After completing a BSc (Hons.) in Chemistry in 2005 she returned to Canada to undertake Doctoral research at the University of Alberta under the supervision of Prof. John Vederas. During her degree Dr. Ross investigated antibacterial peptides called lantibiotics, exquisitely potent molecules that are produced by bacteria as a chemical defense. She received her PhD in Chemistry in 2012 and then joined the lab of Prof. Bradley Moore at the Scripps Institution of Oceanography/University of California at San Diego. At Scripps, Dr. Ross has continued to study peptides from bacteria and her work currently



focuses on how these complex molecules are biosynthesized in nature. Dr. Ross was supported by NSERC during her PhD studies and is currently an NSERC post-doctoral fellow. In addition to federal fellowships Dr. Ross has received multiple University-based awards including a Doctoral Dissertation award from the University of Alberta.

Dr. Ross joins the Department of Chemistry in January 2015.

Best Wishes to Bill Newstead

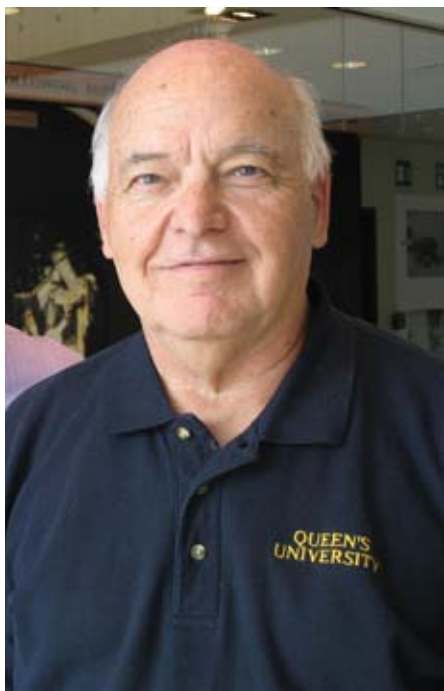
by Michael Mombourquette

William (Bill) Newstead joined our department in 2001, just before we moved into our new digs in Chernoff Hall. Bill came to us after a successful career as a high school teacher and principal in the public school system here in Kingston. He brought with him vast expertise in education, and teaching skills that are rivalled by few today.

Bill's rapport with the students and his teaching ability soon earned him teaching awards and he has won awards in almost every year he has been here. His awards include the Golden Apple Award, the First Year Applied Science Teaching and Learning Award (many times), the Alumni Teaching Award, the Frank Knox Award (twice), the Chancellor A. Baillie Teaching Award. And most recently, he received the Ontario Undergraduate Student Alliance Teaching Award.

Bill first joined the department to teach a few courses and quickly took on more responsibilities. He coordinated our TA day and joined the Chemistry TA Awards Committee to decide which TAs would receive teaching awards each year. He assumed the role of mentor and guide to the tutorial TAs, visiting them in their classrooms and providing valuable insight and guidance to each of the graduate students he advised. I'm sure many of our graduates who now find themselves in teaching roles are relying on some of the guidance offered by Bill when they were here.

Students who have been under Bill's tutelage both in high school and in university hold him in the highest esteem. I have been with Bill several times when we encountered someone from his past who just happened along and who hap-



pily chatted with him and regaled me with stories of their times with Bill as their teacher. Bill seemed to always remember everyone and their names and history as if he had taught them only yesterday – a sign of a great teacher and mentor.

I first encountered Bill as a fellow professor teaching CHEM 112. I have enjoyed working with him over the years, cooperating on CHEM 112 and, more recently, on APSC 131 and 132. Bill is a staunch defender of the students and their educational experiences here at Queen's and we see eye-to-eye on so many issues regarding teaching, even though my skills pale in comparison. Working with Bill

has been a thoroughly enjoyable experience each and every time we have worked together. There are few people I have ever worked with who could match his collegiality and openness when discussing and resolving issues in the day-to-day work world. I have found a friend

and mentor in Bill and I will miss his smiling face and supportive ways. I am sure I am not alone in wishing Bill all the best in his endeavors in the future and I know he will always be welcome here where he can consider himself to be among friends.

Bon-voyage Bill, we'll miss you.

Harrison/MacRae Family Lecture Series

The Chemistry Department thanks the Harrison/MacRae family for a generous gift that will allow the Departments of Chemistry and Physics to jointly host a visiting speaker, in chemical physics or physical chemistry



or a related area, each year.

The fund was established by the estate of the late John Harrison, BComm 1949, and Elizabeth Harrison (Betty MacRae), BA 1949, to “support the costs associated with bringing speakers with an emphasis on chemical physics and physical chemistry” to Queen’s. The Harrison and MacRae families have a long history with Queen’s. Irene MacAllister graduated in 1914 in Honours in Math and Physics, and Alex MacRae graduated in Engineering in 1914. All five of their children went to Queen’s, including Elizabeth Harrison, and many grandchildren are Queen’s graduates as well. This includes Prof. Ian Harrison, a 1981 graduate of the Chemical Physics program, and now with the Department of Chemistry at the University of Virginia.

The Harrison/MacRae lecture will be held each year and the speaker will be chosen by a joint Physics/Chemistry advisory committee. The committee may choose to invite speakers to stay for an extended visit with the goal of enhancing research, scholarship, teaching, or science outreach at Queen’s.

We look forward to the inaugural Harrison/MacRae lecture!

Self-Assembled Monolayers of N-Heterocyclic Carbenes on Gold



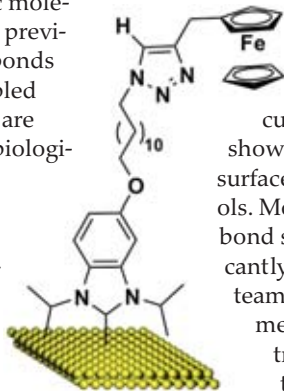
The groups of Drs. Crudden and Horton, in collaboration with Drs. McLean, Wu, Mosey and Kraatz, recently proposed a novel concept for binding organic molecules onto metal surfaces. Their work, published in *Nature Chemistry*, has been garnering quite a bit of attention including a Chemistry World article by Tim Wogan, a Chemical & Engineering News article by Stephen Ritter, and interviews on Station 14 and CKWS.

Why is this work important? Introducing organic molecules to the metal interface results in drastic changes of the surface properties, due to the formation of bonds between the metal surface and the organic moiety. Organic molecules like thiols or thiolates previously known to form such bonds and thiol-based self-assembled monolayers (SAMs) on gold are used in many medical and biological applications, including biosensing and molecular recognition. However, the lack of stability and durability is well known for these systems and this was the main limitation to industrial applications. That is

why an alternative way to anchor organic molecules is highly desirable.

It has been known for the last 20 years that N-Heterocyclic Carbenes (NHCs) can react with metal atoms forming so-called metallorganic compounds with exceptionally strong metal-carbene bonds. Taking into account this fact, Dr. Crudden posed an important question: Is it possible to react NHCs with metal surfaces to translate the properties, in particular the bond strength, robustness, and durability to macroscopic objects?

Drs. Crudden and Horton were able to cover gold surfaces with NHC molecules and scanning tunneling microscope studies performed by Dr. McLean confirm the order of these films on the molecular level. Theoretical calculations performed by Dr. Mosey show that the NHCs bind to the gold surface in a different fashion than thiols. Moreover, calculated NHC-gold bond strength was found to be significantly higher. Indeed, the Queen's team showed that NHC-modified gold metal surfaces demonstrate an extreme durability and are tolerant to a variety of harsh conditions.



In addition, these self-assembled monolayers on gold show considerably greater resistance to heat, moisture, and chemical reagents than their thiol-based counterparts. They are also more oxidatively stable during intensive electrochemical cycling. This opens many plausible applications in the area of electrocatalysis.

A great variety of NHC molecules can be prepared; they can vary sterically and electronically. This will allow for fine-tuning of the packing density on the surface. Moreover, NHC monolayers can be further functionalized after anchoring to the surface to grant access to a variety

of surfaces with desired properties.

Gold surfaces were used for the original experiments due to their biocompatibility, conductivity and ease of handling and purifying. However, Drs. Crudden and Horton are actively working to expand the scope of metals to nickel, copper, and others. Intensive studies on functionalization of metal nanoparticles by NHCs are currently in progress, funded by the Japanese government through Dr. Crudden's satellite lab in Nagoya Japan. Various industrial applications, especially in the areas of metal protection, mining and biosensing are also being explored.

Congratulations to Dr. Tucker Carrington

Dr. Tucker Carrington came to Queen's in 2007 as a Tier 1 Canada Research Chair in Computational Quantum Dynamics. He has established an ambitious research program at Queen's, aimed at developing new tools for computing highly accurate molecular spectra. In 2013/14, his research was recognized with two national awards: the J. C. Polanyi Award for research excellence in physical chemistry, chemical physics, and theoretical and computational chemistry (Canadian Society for Chemistry); and the Gerhard Herzberg Award (Canadian Society for Analytical Sciences and Spectroscopy).

High-resolution spectroscopists are able to measure the position of transitions to great accuracy. Hidden in the data is information on the size, shape, and rigidity of the molecules under study. Theorists compute spectra to predict unobserved transitions and understand energy level patterns. It is possible to combine theoretical and experimental methods to extract more information from observed spectra. For a diatomic molecule such calculations have been routine for decades. New methods for



triatomic molecules were developed about 20 years ago. In the last 5 years the Carrington group has developed new tools that make it possible to calculate vibrational and ro-vibrational spectra of molecules with as many as 10 atoms. This is a difficult undertaking because the motion of atoms may be of large amplitude and the dimensionality of the problem grows with the size of the molecule. The Carrington group has developed several methods for confronting this challenge, all using iterative schemes that require a modest amount of computer memory and processing time.

A Celebration of Professor K.E. Russell's 60 Years at Queen's

By Ralph Whitney

For 60 years Ken Russell has been a colleague, mentor and friend to faculty, staff and students at Queen's. To honour Ken's contributions and to mark this important milestone, the Chemistry Department will be hosting a reception in Ken's honour during Homecoming 2014.

Ken completed both his undergraduate and graduate degrees at the University of Cambridge, the latter under the supervision of Prof. R.G.W. Norrish (Nobel Laureate 1967) studying the cationic polymerization of isobutylene. Following post-doctoral spells at Pennsylvania State and Princeton Universities, Ken joined the Department of Chemistry in 1954 where he developed further interests in radical-mediated processes and their relevance to polymer chemistry. From his arrival in 1954 to his retirement in 1989, Ken also co-authored publications with many of his colleagues including Erwin Buncel, Albert Norris, Jeffery Wan, Brian Hunter, Doug Hutchinson, Don Heyding, Gang Wu, Warren Baker, John Stone and Ralph Whitney.

To acknowledge Ken's many contributions over his 60 years at Queen's, the Department is pleased to host a reception during Homecoming (**Saturday, October 18, 2014, 10 am, Chernoff 117**). Ralph Whitney will give a short reminis-



Professor Ken Russell giving a chemistry demonstration during the 100th Anniversary Celebration of Applied Science (1993).

cence of Ken's research career. Following this, Scott Parent (Eng Chem '91), Hazell Research Professor of Chemical Design and Innovation, Department of Chemical Engineering, will give a short technical presentation on recent developments related to Ken's research interests. Light refreshments will be served in the Walter MacFarlane Smith Family Room at 11 am.

We look forward to seeing you on October 18.

*To mark this occasion, the Department is establishing the **Kenneth Russell Endowed Lecture Series** in polymer chemistry. Fund raising for this initiative will be officially launched at Homecoming, however donations prior to this event may be made at the following link: givetoqueens.ca/Russell.*

Dr. Julia van Drunen

Recipient of the 2012/13 M. Mottashed Graduate Fellowship

Julia grew up in Sudbury, Ontario and moved to Kingston in 2003 to start her BSc in Chemistry with a minor in Geological Science. During her undergraduate studies, she was introduced to research in the laboratory of Prof. Gregory Jerkiewicz where she worked on the corrosion of titanium for medical applications.

After completing her BSc, Julia pursued her curiosity for electrochemistry by entering the graduate program under the supervision of Prof. Jerkiewicz. Her graduate research focused on the development and characterization of nickel and platinum electrocatalysts for energy storage and conversion, as well as the degradation of environmental contaminants. The ultimate goal of this research is to develop electrochemical systems for important processes such as water electrolysis and functional group inter-

conversions that use inexpensive electrocatalysts and environmentally-friendly aqueous solvents. This project included collaboration with Simon Fraser University and the Université de Poitiers in France where Julia spent eight months conducting research with Dr. Teko Napporn and Prof. Boniface Kokoh. In addition to the Marie Mottashed Fellowship, Julia has previously received a McAdie Chemistry Doctoral Student Award, an Ontario Graduate Scholarship, an Electrochemical Society Summer Fellowship, and a Fisher Scientific Tutorial Teaching Award. Besides enjoying ten excellent years as a student and researcher in the Department of Chemistry, Julia initiated and organized the Chemistry "Shinney" Hockey league; a mixed-gender, casual hockey league where students and staff with all skill levels can hit the ice together.

Julia completed her Ph.D. in December of 2013. She is currently a postdoctoral fellow at the Instituto de Química de São Carlos in Brazil. This research institute is a part of the Universidade de São Paulo, which is the foremost research university of Brazil. She is working in the group of Prof. Germano Tremiliosi-Filho and supported by the state of São Paulo with a FAPESP postdoctoral fellowship. Her current research is geared towards the development of electrochemical processes for the treatment of waste materials from Brazil's booming bioethanol industry. With this position she hopes to maintain strong ties to the Department of Chemistry at Queen's and assist Prof. Jerkiewicz with research collaborations and educational exchanges with the Universidade de São Paulo.



Jeremy Durelle

Recipient of the Christopher Knapper Teaching Award



Jeremy Durelle is originally from Fredericton, New Brunswick. Staying close to home, he completed an undergraduate degree at UNB, with a double major in physics & chemistry (Hons). After completing his BSc, he moved to Kingston to pursue a master's degree in

astrophysics. His master's work focused on developing a theoretical model that could explain strange features of edge-on spiral galaxies. He joined Dr. Philip Jessop's group for doctoral work, with a project aimed at developing a mathematical description of switchable hydrophilicity solvents (SHS). By having a working mathematical basis, he can optimize the switching process and allow for a large range of solvents to qualify as SHS. He is currently writing his thesis and plans to be finished by the end of the summer.

In addition to the Knapper teaching award, Jeremy previously won the "Friends of Chemistry" TA award. He notes that he is passionate about teaching and he enjoys coming up with efficient and effective teaching methods.

TA Teaching Awards

Promoting and recognizing excellence in teaching (tutorial and laboratory) by Teaching Assistants in Chemistry



TA Award recipients (left to right): Mark Raycroft, Fisher Scientific Teaching Assistant Award for Chemistry Tutorials; Kourosh Purdavaie, David Thomas Teaching Assistant Award for Synthetic Laboratory; Nausheen Sadiq, William Patrick Doolan Prize in Chemistry; Jeremy Durelle, Friends of Chemistry TA Award for Excellence in Teaching; Matthew Thompson, Din Lal Teaching Assistant Award

Science Rendezvous

by Gillian Mackey

On May 3, members of the Department of Chemistry participated in Kingston's fourth annual Science Rendezvous, a day of scientific engagement and education for the community. The day was very well-attended, with approximately 3500 visitors to the K-Rock Centre. Dr. Michael Mombourquette presented a chemistry magic show, along with Prashant Agrawal, Marie Barnes, Sean Mombourquette, Nausheen Sadiq, Lisa Saunders, Christene Smith, Samantha Voth, and Chris Ziebenhaus. Dr. Hans-Peter Loock and his students, Nicholas Andrews, Amy MacLean, John Saunders, Sean Takahashi, and Michaela Thomas demonstrated the science of lasers. Visitors were also able to try hands-on chemistry with Tham Adhikari, Mona Ashrafkhorasani, Brian Bestvater, Lily Huang, Gillian Mackey, Lili Mats, and David Simon.



We are pleased to announce that the following speakers have been confirmed for our 2014-2015 Seminar Series. For more information and dates, please visit our website at www.chem.queensu.ca/chemistryN/About/seminarseriesN.asp



Prof. Robert Waymouth, Stanford University, USA
Prof. Dongling Ma, Institut National de la Recherche Scientifique, Quebec
Prof. Chris Braddock, Imperial College, England
Prof. Chris Baddeley, University of St. Andrews, Scotland
Prof. James Green, University of Windsor, Ontario
Prof. Daniel Armstrong, University of Texas at Arlington, USA
Dr. Ewa Dabek-Zlotorzynska, Environment Canada, Ontario
Prof. François Lagugné-Labarthe, Western University, Ontario
Prof. Bruce Arndtsen, McGill University, Quebec
Prof. Eric Rivard, University of Alberta, Alberta
Prof. David Perry, University of Akron, USA
Prof. Timothy Swager, Massachusetts Institute of Technology, USA
Prof. Gilbert Walker, University of Toronto, Ontario
Prof. Arturo Orellana, York University, Ontario
Prof. Jay Switzer, Missouri University of Science and Technology, USA
Prof. Edward Valeev, Virginia Tech, USA
Prof. Graham Cooks, Purdue University, USA
Prof. David MacMillan, Princeton University, USA
Prof. Gary Molander, University of Pennsylvania, USA

Congratulations to the Class of 2014!



Front Row (from left): Nicole Grenon, Tia Anderlini, Kate Henderson, Valerie Chiykowski, Jaida Williamson, Vidya Hemraj, Rhea Ramachandran, Joelle Becker, James Payne
Back Row (from left): Mei-Ni Belzile, Alexander Jardine, David Tom, Rebecca Hall, Alexander Ford, Kate Mill, Regan Sedgewick, Yunjung Oh, Kevin Cummings, Cherise Cadore, Dylan Glancy, Jason Rygus

Undergraduate Life

by Tia Anderlini

It was a very busy year for the Chemistry Department Student Council (DSC). The DSC is made up of a group of undergraduate chemistry students with the primary goal of holding social events in the department and fundraising for the year-end Chemistry banquet. Such social functions this year included a welcome BBQ in September, Chemistry clothing sales, a pumpkin carving contest and pumpkin pie sales on Halloween, pizza and bake sales, Valentine's cookie sales, and social outings. This year's banquet was held at The Delta Waterfront Hotel and was well attended with over 100 guests! Awards for Professor, TA, and Staff of the Year were presented to Nick Mosey, Mark Raycroft, and Françoise Sauriol, respectively. In addition to social activities, the DSC held two information

sessions for undergraduates: "Working in the Department", which provided chemistry and biochemistry students with information on the jobs available in the department during the summer as well as an outline of the application process, and "Fourth-Year Thesis Projects" to give third-years an idea of what to expect for their upcoming honours projects. A DSC representative was also present at the Queen's Open House to answer the questions of prospective students. Finally, administrative tasks such as conducting teaching assessments, and meeting with the other DSCs of Queen's in DSC Assembly and Faculty Board were also carried out by the DSC. This year was a blast for the DSC and would not have been as successful if not for our hard working crew!

Graduate Student Life in the Department

by Tamara de Winter

It has been an exciting year for the Queen's Graduate Chemistry Society (QGCS). The QGCS worked hard throughout the year to provide social, educational and charitable events.

Last summer, as always, we started with departmental lunch-time barbecues. We had movie nights where we showed films in a seminar room and provided popcorn. The Graduate Society also hosted a guest seminar speaker, Prof. Guy Bertrand, who was invited by the graduate students of the department. We ended the summer with a QGCS golf tournament. In the Fall, we held several welcome mixers for the incoming students, a barbecue for the annual Queen's Graduate Chemistry Symposium, and a career workshop with members of the Queen's Chemistry Innovation Council. This workshop provided a wealth of knowledge of industrial life, careers in chemistry and the exciting networking opportunities. The graduate students also organized a team for Run for the Cure, raising money by providing coffee and treats in the department. Likewise, we volunteered to provide barbecues and departmental tours for the alumni during the Homecoming weekends. National



Chemistry Week was celebrated later in the Fall, with different events each day: chemistry trivia and pizza; a periodic table of cupcakes with morning coffee; a pumpkin carving competition; and we finished with a Halloween social. At the end of November, our annual holiday party was held at *Megalos*. This holiday party was the most successful yet!

During the Winter term, the Graduate Society continued to provide movie nights and organized a bowling event at *Cloverleaf Lanes*. In the end, the QGCS had a successful year and was able to create two new positions in the society: a Sports Rep and a Union Rep.

The 2013/2014 elected QGCS executive are: Tamara de Winter, President; Yoseif Makonnen, VP Internal Affairs; Kyle Boniface, VP Finance; Nausheen Sadiq, VP External Affairs; Prashant Agrawal, Sports Rep.; XiMing Zhu, Union Rep.; Nakkiran Arulmozhi, 3rd Floor Rep; Danielle Macoretta, 4th Floor Rep; Marie Barnes, 5th Floor Rep.



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