A Green Solution to Industrial Fumes
By: Lakshman Rajanathan and Mohammad Raza

Using new and innovative methods to solve the air pollution produced by industrial fumes.

A More Sustainable Approach to Synthesis and Deposition of a Simple and Robust Coating for Thrombosis Prevention
By: Kiril Fedorov, Christophe Blaszykowski, Sonia Sheikh, and Michael Thompson

Exposure of synthetic materials to body fluids may result in undesirable protein−material interactions that can potentially trigger deleterious biological processes such as thrombosis. The result is increased chances of heart attack, stroke, or other cardiovascular complication after extravascular blood procedure. The coating was done on wide variety of materials including: several common plastics, metals and other types of materials used in the medical industry. Several of the coated materials (PVC, PC, steel 361) were tested directly for their compatibility with whole human blood. Antithrombogenicity was assessed after 2,5,10 and 60 min, 3 hours, 6 hours exposure to whole human blood dispensed at a shear rates of 1, 300, 900, 1000 and 1500 s^{-1}. Overall the coating had shown reduction at ~90% or more in adhesion and clot formation on all times and shear rates. For the synthesis of the coating for a more sustainable approach the Pfizer solvent guide was used with majority of early undesirable solvents replaced with desirable solvents. Overall the coating proved to be robust on wide variety of materials and has shown very high potential in blood compatibility when used with more preferred solvents from Pfizer solvent guide comparable to original work.

Asymmetric Hydrogenation by NHC-stabilized Borenium Ion Catalysis
By: Jolie Lam and Douglas W. Stephan

Amines and their derivatives are synthetically important compounds with a wide range of applications, varying from dyes to pharmaceuticals. In particular, potential pharmaceutical intermediates and targets are required in high enantiopurity, which is typically achieved by chiral transition metal-mediated transformations.[1] N-heterocyclic carbene (NHC)-stabilized borenium ions[2] have recently been reported to be excellent metal-free catalysts for the hydrogenation of imines under mild conditions by Stephan and coworkers. We are now targeting the syntheses of new borenium ions that incorporate chiral substituents for the enantioselective hydrogenation of prochiral imines. Borenium cations stabilized by chiral bisoxazoline[3] carbenes were synthesized and preliminary results show excellent catalysis with high conversions. Simultaneously, we are tuning the Lewis acidity and selectivity of these systems by exploiting variations of the borane to enhance reactivity.[4] The efficacy of these systems in the asymmetric catalytic reduction of ketimines will be discussed.

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3. Lindsay, D. M.; McArthur, D. Chem. Commun. 2010, 46, 2474-2476.
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Catalytic Reduction of Phosphine Oxides to Phosphines by Electrophilic Phosphonium Cations (EPCs)

By: Meera Mehta, Isaac Garcia, Manuel Perez, and Doug Stephan

Phosphorus compounds have been traditionally thought of as Lewis donor ligands used in transition metal and organometallic chemistry. Such ancillary roles have been critical to a number of landmark advances in catalysis. However, phosphorous based Lewis acids have been studied to a less extent. Previously, the Stephan Group reported the preparation and Lewis acidity of electrophilic phosphonium cations $[(C_6F_5)_3PF]^+$and $[(SIMes)PFPh_2][B(C_6F_5)_4]_2$ and the application of these species in the hydrodefluorination of fluoroalkanes, the isomerization of terminal olefins, and hydrosilylation of alkenes, alkynes, imines and ketones . This reactivity has been attributed to their energetically accessible σ*(P−F) acceptor orbitals. In this presentation, the catalytic reduction of phosphine oxides to phosphines will be discussed.

Chemical Analysis and SEM Imaging of the McAbee Fossil Beds

By: J Matt Miller and Dr. Nancy Van Wagoner

McAbee fossil beds is an understudied Eocene Epoch fossil site near Cache Creek, BC. During a recent trip to the fossil beds an interesting geological structure was discovered. At the center of this geological structure were unique minerals and the morphology of these minerals was distinct from the surrounding fossil beds. The assumption was that these minerals were derivatives of Gypsum, which had been found in large quantities around McAbee previously. The scanning electron microscope/ energy dispersive x-ray detector at Thompson Rivers University was employed for imaging and total elemental analysis. Upon chemical analysis it was discovered that we were entering the world of Iron Sulphate minerals. These minerals are often hydrated and hydrous, making study of them difficult. These minerals come in a variety of morphologies with only small differences in chemical composition present between mineral species. Iron Sulphates are of environmental importance due to being associated with acid mine drainage and associated to a lesser extent with volcanic fumaroles. The SEM/EDS technique provides a rapid detection of these Iron Sulphate minerals, with analysis of these minerals at the McAbee site ongoing.

Determination of Parabens in Hair Care Products by Liquid Chromatography – Mass Spectrometry

By: Trevor Johnson, Dr. Kingsley Donkor, and Dr. Sharon Brewer

This experiment attempted to analyze the presence of three species of parabens in shampoo samples obtained from various hotels. Parabens are effective preservatives that are widely used in cosmetic products to fend off microbial organisms. Research has suggested that parabens have estrogenic effects and are found in the bodily tissues of breast cancer patients. Shampoo samples were mixed and diluted with a methanol solvent and analyzed using liquid chromatography – mass spectrometry (LC-MS). The methods used in this experiment were derived from previously optimized studies on parabens in solid cosmetic foundations. External standards of methyl, ethyl, and

butylparabens were first used for analysis; internal standards of the same compounds were later used to test and validate the results obtained by the external standard analysis. Some preliminary results were found using external standards, but the results obtained by internal standards indicated that the desired analytes were not efficiently extracted from the shampoo matrix, meaning that the results obtained remain inconclusive.

Does Walking "Waste" Gas?
By: Leah Ellis

“The energy needed to produce the food you would burn (from a typical American diet) in walking a given distance is greater than the energy needed to fuel your car to travel the same distance” claims John Robbins in his bestselling book, Diet for a New America. This poster evaluates John Robbins' claim, calculating and comparing the carbon footprints of various transportation and dietary lifestyle choices. While it is concluded that walking does not in fact “waste gas”, the results of this calculation highlight large differences in carbon footprints between urban lifestyle choices. The question “does walking waste gas?” raises awareness and inspires critical thinking.

Finite-temperature Investigation of Heterogeneous CO_2 Reduction over $In_2O_{3-x}(OH)_y$ from First Principles
By: Mireille Ghoussoub and Chandra V. Singh

In light of climate change and growing global energy demands, the conversion of greenhouse gas CO_2 into fuels offers a promising path to building a carbon neutral economy. The production of such sustainable fuels, termed “solar fuels”, has led to a widespread investigation by the scientific community to find a cheap and abundant catalyst material capable of efficiently splitting CO_2 . The chemical concept of “Frustrated Lewis Pairs” (FLPs), in which a sterically hindered Lewis acid-base pair forms a highly reactive site conducive to the activation of small molecules, may offer an effective solution to CO_2 reduction. Recently, FLP sites on the surface of hydroxylated indium oxide nanoparticles have been demonstrated to assist in the Reverse Water Gas Shift (RWGS) reaction by heterolytically splitting H_2 and subsequently enabling CO_2 reduction. However, the thermal-sensitivity of the reaction requires an understanding of the fundamental interplay between surface FLPs, temperature, and its consequences for the RWGS mechanism. Metadynamics is a computational tool to improve the efficiency of ab initio molecular dynamics (AIMD) simulations by introducing energy biases to explore the relevant parts of reaction free energy surfaces. Here we use Metadynamics-biased AIMD to obtain the free energy and scape of the RWGS reaction at finite temperature. The reaction is simulated at 20 °C and 180 °C and the minimum energy reaction pathways and energy barriers corresponding to H_2 dissociation and CO_2 reduction are obtained. We also present a correlation between temperature conditions and surface FLP reactivity.

Friedel-Crafts Benzylation Catalyzed by Highly Lewis Acidic Phosphonium
By: James H. W. LaFortune, Jiangtao Zhu, Manuel Pérez, and Douglas W. Stephan

Fridel-Crafts alkylation, wherein a Lewis or Brønsted acid catalyzes carbon-carbon bond formation, endures as the preferred method of arene and heteroarene alkylation in many industries since its discovery in 1887. Over the past several decades, significant efforts have been made to lower catalyst loadings and expand the substrate scope. While catalytic Fridel-Crafts alkylations with benzylic alcohols are well known, alkylations with benzylic ethers are somewhat less common. Furthermore, these reactions generally require high catalyst loadings of 5 to 10 mol%. Recently, we have developed a new class of Lewis acids based on highly electrophilic phosphonium cations. These species have been shown to be highly reactive, facilitating these reactions with low catalyst loadings. In this poster we explore the reactivity of one such Lewis acid towards Friedel-Crafts alkylations with benzylic alcohols and ethers.

Green Chemistry Research at Prof. Wei Zhang's Lab at UMass Boston
By: Shuai Liu, Xin Huang, Xiaofeng Zhang, Asha Kadam, and Wei Zhang

UMass Boston lunched the first PhD in green chemistry program in 2002 by Prof. John Warner. It also established a Center for Green Chemistry to integrate research, education, and collaboration on green chemistry. As the Director of the Center, Prof. Wei Zhang's lab is focused on the development of greener technologies for organic synthesis, organocatalysis, and medicinal chemistry. New synthetic methodologies based on fluorous synthesis, multicomponent and cascade reactions, and recyclable organocatalysis have been applied to the synthesis of biologically interested molecules. This poster covers our recent effort on solution-phase synthesis of drug-like molecules with diverse scaffold and asymmetric synthesis of fluorine-containing molecules with multiple stereocenters. Discovery of new and potent bromodomain inhibitor UMB32 which was prepared by a two-step synthesis will be highlighted. Another project sponsored by ACS Green Chemistry Institute Pharmaceutical Roundtable on solvent screening for Grignard reactions is also highlighted.

Join the Network of Early-Career Sustainable Scientists & Engineers
By: Natalie O'Neil and the Network of Early-Career Sustainable Scientists & Engineers

The Network of Early-Career Sustainable Scientists and Engineers (NESSE) is an international community of academic researchers and young professionals in the first ten years of their career working on technological solutions to today's most pressing environmental and energy challenges. We envision a prosperous and sustainable future for all, facilitated by collaborative and green approaches to science and technology. Our mission is to inspire and mobilize a new generation of interdisciplinary scientists and engineers who strive to achieve a more sustainable future.

Method Development for the Determination of Haloacetic Acids in Drinking Water
By: Stephanie Wright and Dr. Sharon Brewer

Disinfectants are added to drinking water in order to remove pathogens, remove taste and colour, prevent algae growth in sediment basins, and improve the efficacy of coagulation and filtration. Free chlorine is the most popular disinfectant because of its low cost as well as its relative low oxidizing potential, which leads to lower residual chlorine in the water. Reactions of chlorine and the naturally occurring organic matter in water leads to disinfection by-products. High levels of disinfection by-products have been linked to birth defects and cancer, and must therefore be monitored in water treatment and distribution systems. In this research, the United States Environmental Protection Agency (US EPA) standard method 552.2 was optimized for analysis of drinking water in Kamloops British Columbia. The method developed was then applied to determine concentrations of one class of the disinfectant by-products, haloacetic acids in drinking water. The method was efficiently optimized and all samples tested were found within the regulatory limits of Health Canada.

New Unsymmetrical Iron(II)PNNP' Asymmetric Transfer Hydrogenation Catalysts
By: Samantha A.M. Smith and Robert H. Morris

Enantiomericaly pure alcohols are used in the pharmaceutical and fine chemical industries and are generally obtained via reduction of prochiral ketones using complexes based on precious metals. It is highly desirable to replace these precious metals to make efficient and inexpensive catalysts for this reaction and is a long-standing goal to use non-precious, Earth-abundant metals such as iron. This poster will focus on new iron complexes synthesized with varying steric and electronic properties. It was achieved using a modular synthesis developed in our lab.

Nicotine-derived Ammonium Salts as Highly Efficient Catalysts for Chemical Fixation of Carbon Dioxide into Cyclic Carbonates Under Solvent-free Conditions
By: Yasaman Heidari, Abdol R. Hajipou, and Gholamreza Kozehgary

Nowadays, the development of catalytic processes for the efficient utilization of naturally abundant carbon dioxide, one of the greenhouse gases, has drawn much attention. One of the few commercial synthetic processes utilizing CO_2 as a raw material is the insertion of CO_2 into epoxides to produce five-membered cyclic carbonates. A series of easily prepared nicotine-derived ammonium salts were applied for the first time as recyclable and efficient catalysts for the coupling of carbon dioxide and epoxides to form cyclic carbonates at low pressure without using any organic solvents and co-catalysts. Remarkably, excellent yields and selectivity were achieved when 1-benzyl-1-methyl-2-pyridin-3-yl-pyrrolidinium bromide [MBNT]Br was used as the catalyst. Furthermore, the catalyst can be easily recovered and reused without a significant loss of activity.

Sustainable Plasmonic Nanoarchitectures
By: Osai Clarke and Christa Brosseau

Plasmonic nanostructures that are uniform in size, shape, and polydispersity are highly desirable for many applications, including plasmon-enhanced solar cells and localized surface plasmon resonance (LSPR) sensing. Unfortunately, such structures are often difficult and costly to fabricate, which limits their widespread application. Therefore, there is great interest in sustainable plasmonic architectures which can be manufactured using low cost fabrication strategies, as well as earth-abundant metals. In this work, we will present our recent progress towards the development of sustainable plasmonic architectures for a variety of applications, including rapid diagnostics and surface-enhanced Raman spectroscopy (SERS) sensing.

The Hazard Reflection Framework
By: Kile McKenna and Dr. Sharon Brewer

The Hazard Reflection Framework is a tool developed at Thompson Rivers University (TRU) to evaluate the sustainability of undergraduate experiments. An experiment is scored by assessing a penalty for each hazard statement required under the Globally Harmonized System of Classification and Labeling of Chemicals (GHS) for all chemicals used. A penalty point score is generated and combined with the number of students completing the experiment in a typical year to generate a hazard cost score. To give context to the penalty point and hazard cost scores, and to further incorporate principles of green chemistry, assessment is completed considering the scale, waste generated, and energy and water consumed by the experiment. The educational benefits of performing the experiment are then evaluated with respect to the costs discussed, and all of the information is incorporated into an information graphic. The Hazard Reflection Framework has two intended purposes: it is designed to aid educators in assessing the sustainability of teaching experiments and is intended to serve as an in-class tool to promote discussion about applying green chemistry principles to experiments familiar to the students. This poster presents the basis for the Hazard Reflection Framework and shows its application through TRU case studies.

Waterproof Strong Chitosan Plastic
By: Becky Winnick, Thanh-Dinh Nguyen, and Mark MacLachlan

Conventional plastic products are made from petroleum, a non-renewable resource. The products are non-biodegradable and often contain compounds that are toxic to creatures on Earth, including humans. Even recyclable plastic can only be "downcycled," so it all eventually becomes persistent pollution. A newer bioplastic that is made from corn is biodegradable and renewable, but its production requires resource-intensive agriculture. Chitosan bioplastic, on the other hand, can be made from waste material - discarded crab and shrimp shells. Previous research has successfully produced strong chitosan bioplastic, but swelling and poor stability in water remain a challenge. Now, we have developed a facile new method to create chitosan bioplastic that remains strong even

after soaking in boiling water. The additional antibacterial and wound-healing properties of chitosan make this material promising for application in food packaging and healthcare.