

### *Minimizing the Copper Leaching in CuAAC Reactions by a Thin Carbon Shell on Cu-Fe Microparticles*

By: [Mary Bateman](#), Mitra Masnadi, Peng Zhao, Olivia Trautschold, Nadi Braidy, Bruce Koel, and Audrey Moores

Nano-sized, magnetically recoverable catalysts are attractive options for heterogeneous catalysis due to 1) reactive surface area from its nanosize, leading to good catalytic activity; 2) magnetic properties, allowing for ease of separation for catalyst removal; and 3) heterogeneity, implying the active catalytic species is not lost as readily as its homogeneous counterpart. Previously, we have shown copper-coated iron microparticles (Cu-Fe MPs) can catalyze Cu(I)-catalyzed alkyne azide cycloaddition reactions (CuAAC), specifically of biologically relevant molecules. To further improve the heterogeneous nature of our catalyst, these particles were coated with carbon at the surface (C@Cu-Fe MPs) with the intention of decreasing both physical and chemical loss of copper into the reaction. While the carbon coating was effective in decreasing the loss of Cu, it was also found to be linked to an increase in reaction time.

### *Development of Novel 3,5-Dimethylisoxazoles Bromodomain Inhibitors*

By: [Shuai Liu](#), Michael R. McKeown, Harry Fu, Dennis L. Buckley, Jun Qi, James E. Bradner, and Wei Zhang

Bromodomains (BRDs) are a class of epigenetic reader proteins which recognize acetyl-lysine marks on chromatin. These proteins frequently participate in oncogenic translocations and amplifications in a variety of cancers. Inhibition of bromodomains with small molecules has recently been proven to be a powerful tool in the study of chromatin biology. Using pioneering, fluororous multicomponent reactions we have rapidly developed a chemical library of bromodomain inhibitors around a 3,5-dimethylisoxazole biasing element with an initial biochemical IC<sub>50</sub> of 16  $\mu$ M. A robust chemical screening and development program has allowed rapid optimization of novel BET bromodomain inhibitors around an imidazo[1,2-a]pyrazine scaffold. Lead compound UMB-32 shows 637 nM biochemical potency and 724 nM cellular potency in BRD4-dependent lines.

### *Catalytic Formylation of Primary/Secondary Amine with CO<sub>2</sub> and H<sub>2</sub>*

By: [Mohammad A. Affan](#) and Philip G. Jessop

Catalytic hydrogenation of CO<sub>2</sub> is an efficient and selective way to form value added fine chemicals such as formic acid derivatives, but most of the highly active catalysts have required precious metals. Herein, we describe the hydrogenation of CO<sub>2</sub> to formamide using a primary/secondary amine in the presence of [MX<sub>2</sub>(dmpe)<sub>2</sub>] (M = Fe(II) and Ni(II); X = CH<sub>3</sub>CO<sub>2</sub>-; acac-; dmpe = 1,2-bis(dimethylphosphino)ethane) as catalysts in DMSO. Morpholine and 2-ethylhexylamine are formylated at 100 °C and 135 °C, respectively, at a total pressure of 100 bar. Morpholine was formylated with a TON up to 18,000, which is approaching the range of TON values reported for noble metal-phosphine complexes. 2-Ethylhexylamine formamide

obtained with a TON 1,600 has been described for the first time. With the appropriate selection of catalyst and reaction conditions, >90-98% conversion of amine was achieved to form a formamide. In this study, the effect of the changing the metal to amine ratio has been investigated.

*Synthesis and Characterization Of Biochars Made From Anaerobically Digested Food Wastes For Water Remediation.*

By: Dr. Thamara Laredo and [Nawal Almalki](#)

Several studies have shown that Biochar are effective in the absorption of contaminants. A set of studies in particular has shown that anaerobically digested substrates make biochars that have higher surface area and sorption capacity towards certain molecules. . In this study waste from the beer industry will be used as the biomass from which biochars will be made. This waste has been anaerobically digested and can be acquired easily from a local brewery. The substrate will be processed by pyrolysis at 600°C in a reductive atmosphere. The resulting biochar will used to absorb trichloroethylene (TCE) and phosphates in water. The removal of both TCE and phosphates are locally relevant. First, the Lake Simcoe Clean Up Act has decreased the maximum acceptable loads for phosphates from wastewater treatment plants from 0.3 to 0.1 mg/L. Second, TCE is the main contaminant present in a controversial brownfield site in the city of Orillia which has cost the city over 100 million dollars in assessments and monitoring. It is expected that this research will contribute towards the possible remediation of these issues as well as helping with the recycling of an otherwise useless waste.

*Perovskite Thin Films for Potential Solar Cell Application: A Study on Film Degradation*

By: [Catherine Tran](#) and Yi Liu

Organometal trihalide perovskite thin films have recently emerged as a very promising candidate for use in harvesting solar energy. One major concern, however, is the sensitivity of the films to moisture in the air, leading to quick degradation of the perovskite films. We observed the degradation behaviour of specifically vapour-deposited methylammonium lead triiodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) perovskite films over time, and seeing the effect of applying another material film, namely N,N'-Di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB), to encapsulate perovskite for protection, at 10, 20 and 30 nm of thickness. X-ray diffraction analysis and subsequently calculated integrated intensity ratios of diffraction peaks visualized evident degradation of perovskite film over time. From data obtained, it is clear that an encapsulation layer such as NPB has a significant impact in protecting perovskite film as a moisture barrier, under limited UV light exposure, and at ambient temperature and relative humidity conditions. Modelling showed best match of experimental data with the Avrami equation, reflecting phase transformation occurring in the perovskite film into its decomposition

products, lead iodide ( $\text{PbI}_2$ ) and methylammonium iodide ( $\text{CH}_3\text{NH}_3\text{I}$ ). Though further work in experimenting with other possible materials is needed, NPB offers promise in being a candidate encapsulation material, showing that perovskite film degradation can be overcome.

### *A Single-Component Photocatalyst for Gas-Phase $\text{CO}_2$ Reduction: Toward Efficient Solar Fuel Production*

By: [Laura B. Hoch](#), Thomas E. Wood, Paul G. O'Brien, Kristine Liao, Laura M. Reyes, Charles A. Mims, and Geoffrey A. Ozin

The solar-to-chemical energy conversion of the greenhouse gas,  $\text{CO}_2$ , into carbon-based fuels is a very important research challenge, with implications for both climate change and energy security. We have experimentally identified key attributes of hydroxylated indium oxide nanoparticles,  $\text{In}_2\text{O}_{3-x}(\text{OH})_y$ , that function in concert to reduce  $\text{CO}_2$  under simulated solar radiation.  $\text{In}_2\text{O}_{3-x}(\text{OH})_y$  nanoparticles are prepared with varying surface hydroxide and oxygen vacancy content to investigate the effects of these parameters on light-driven, gas-phase  $\text{CO}_2$  reduction rates. By optimizing these parameters,  $\text{CO}_2$  can be converted to CO, in the presence of  $\text{H}_2$ , at a rate as high as  $0.60 \mu\text{mol gcat}^{-1} \text{hr}^{-1}$  under 0.8 suns of simulated solar irradiation at  $150^\circ\text{C}$ .  $^{13}\text{CO}_2$  isotope labeling experiments identify CO as the sole carbon product of  $\text{CO}_2$  photocatalytic reduction. Significantly, the surface hydroxide and oxygen vacancy concentrations correlate well with the  $\text{CO}_2$  adsorption capacity and CO production rate, suggesting both play a key role in the reaction mechanism. This research provides insight towards the rational design and optimization of single-component gas-phase  $\text{CO}_2$  reduction photocatalysts to be incorporated into current advanced systems for solar fuels generation.

### *Modified Chitosan Beads With Different Cross-linkers for Phosphate Removal from Aqueous Solution*

By: [Mohammad Mahaninia](#) and Lee D. Wilson

Adsorption of phosphate from aqueous solution on different cross-linked chitosan beads was investigated in batch mode. The effect of different cross-linker and its concentration on modification of chitosan beads were also investigated. Isotherm Sips was used to fit the equilibrium data, whereas the pseudo-second-order equation was used for the kinetic data. The sorbents were characterized by elemental analysis, TGA, SEM and FTIR. The results show that chitosan bead cross-linked with Epichlorohydrin has a better sorption toward phosphate ions.

### *Phosphonium/Aminosilane Frustrated Lewis Pairs for Carbon Dioxide Reduction*

By: James LaFortune, Thorsten vom Stein, and Douglas W. Stephan

Frustrated Lewis pairs (FLPs) were first discovered in 2006 when the reactivity of some bulky Lewis acid/base pairs were shown to remain unquenched due to steric and electronic effects, leaving them free to activate a variety of small molecules. FLPs have been shown to react with dihydrogen, N<sub>2</sub>O, and CO<sub>2</sub> among a number of others and can be used to catalyze the hydrogenation of bulky imines, enamines, enol ethers, alkenes, and aldehydes. Reactivity of FLPs with CO<sub>2</sub> has been investigated for a variety of systems achieving both stoichiometric and catalytic reductions. 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. In this poster we explore the reaction of these Lewis acids with CO<sub>2</sub> and aminosilane substrates.

### *Electrophilic Phosphonium Dications Derived From Pyridine and Ferrocene Scaffolds*

By: Julia M. Bayne, Ian Mallov, Michael H. Holthausen, Meera Mehta, and Douglas W. Stephan

Until recently, main group Lewis acid catalysts rarely featured group 15 atoms as Lewis acidic active sites. In the past decade, however, the Lewis acidity of particularly the heavier group 15 elements has been harnessed for a range of stoichiometric and catalytic transformations. Our group has recently demonstrated that phosphorus-based Lewis acids as catalysts can catalyze difficult transformations such as hydrodefluorination of fluoroalkanes, hydrosilylation and transfer hydrogenation of alkenes and deoxygenation of ketones. One way we have increased the Lewis acidity of phosphorus in phosphonium cations is by adding a second positive charge. Herein we present two approaches to synthesizing phosphonium dications, and their stoichiometric and catalytic reactivity.

### *Pesticides and Oxodegradable Agriculture Mulch*

By: Kayla Snyder

Agriculture mulch films made from polyethylene are known to have many benefits for the agriculture practice including increased yields and resource efficiency. In accordance with the tenth principle of green chemistry which states “Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment” these films can be designed to be oxo and bio degradable at the end of the season by “programming” them to last for a desired period of time. However, when pesticides are applied to these films the degradation of the films may be affected. This research will begin to fill the large gap on the effect of pesticides applied onto degradable polyethylene mulch. It is important to address this gap as crops covered with mulch films made from polyethylene require

much less pesticides than un-mulched crops to produce the same or higher yields however recommendations for using pesticides and plastic mulch films together are limited. It is hoped that research will effectively lower the dependence on pesticides for crop development.

### *Synthesis of 3-Acetamido-5-acetylfuran From N-Acetyl-D-glucosamine Using Ionic Liquids*

By: Yi Liu and Francesca M. Kerton

Chitin can be obtained from the shells of crustaceans (i.e. shellfish waste), and is the most abundant biopolymer in the ocean. N-acetyl-D-glucosamine (NAG), a sugar, is the monomer of chitin. Controlled dehydration of NAG can generate a new compound, 3-acetamido-5-acetylfuran (3A5AF). This is the first nitrogen-containing product obtained from the dehydration of a hexose in solution, and we hope that it can act as a platform chemical for a series of substances. We are interested in the synthesis of 3A5AF from NAG using a series of ionic liquids ([Bmim]Cl, [Bmim][HSO<sub>4</sub>], [Bmim-SO<sub>3</sub>H][HSO<sub>4</sub>] etc.). The function of additives (sodium salts and boric acid), and extracting solvents (EtOAc, 2,5-Me-THF, MIBK and alcohols) has also been studied. The reaction was conducted under different conditions including conventional heating and microwave irradiation. The reuse of starting materials (NAG and additives) and ionic liquid ([Bmim]Cl) was tried. Mechanistic studies have also been performed and important intermediates were detected. Factors that may influence 3A5AF yields were investigated, such as the solubilities of NAG and the acidities of the systems. Some physical and chemical properties of 3A5AF have been studied and will be useful in future applications.

### *Synthesis of Highly Ordered Mesoporous BiOBr-Bi<sub>2</sub>WO<sub>6</sub> Nanosheet Composites with Efficient Photocatalytic Activity*

By: Mingshan Zhu, Liqun Qiu, Cheng Lu, M. Cynthia Goh

We present a facile template hydrothermal route for the preparation of highly ordered mesoporous BiOBr-Bi<sub>2</sub>WO<sub>6</sub> nanosheets composites in the presence of bismuth nitrate, bismuth nitrate, cetyltrimethyl ammonium bromide (CTAB) as precursors. The XRD spectra exhibit that an ordered structure with 2.5 nm pore is formed in the as-prepared nanocomposites. The highly ordered mesoporous structures could be clearly seen by the TEM images. Moreover, compared to the non-mesoporous structures, the as-prepared highly ordered mesoporous BiOBr-Bi<sub>2</sub>WO<sub>6</sub> nanosheets display higher catalytic performance for photodegradation of RhB pollutants under visible light irradiation.

## *Ruthenium complexes for chemical and solar energy applications*

By: Demyan E. Prokopchuk, Molly M. –H. Sung, Robert H. Morris

A growing concern over an ever-increasing reliance on fossil fuels has sparked an interest in the development of renewable energy. Furthermore, greenhouse gas emissions from the use of fossil fuels and the resulting environmental impact have caused many researchers to investigate “greener” forms of energy. Solar power provides realistic means of sustainably meeting our energy demands;<sup>1</sup> however, it typically requires a second conversion from electrical energy into chemical potential energy due to the intermittent nature of sunlight. Following a report in 2009 by Milstein and coworkers in which a Ru-PNN pincer complex photochemically produced H<sub>2</sub> and O<sub>2</sub> from water,<sup>2</sup> we report a Ru-NCN metal-ligand cooperative system that demonstrates the intramolecular cleavage of O-H bonds upon coordination to water.<sup>3</sup> This initial observation of O-H bond cleavage is a key step toward the design of photocatalysts that can directly convert sunlight into H<sub>2</sub> gas for use as fuels.

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## *Silicon Nanocrystal Research in the Geoffrey Ozin Research Group at the University of Toronto*

By: Wei Sun, Chenxi Qian, Kenny Chen, Melanie Mastronardi

Silicon nanocrystals possess unique optical and optoelectronic properties that vary predictably with crystal size and surface capping, which means can be they tailored to suit specific requirements for use in various applications. Because silicon nanocrystals have the advantage of being purportedly less toxic, earth abundant, and relatively inexpensive compared to archetypal heavy metal nanocrystals like CdSe and PbS, our group has dedicated considerable effort to the development of this field of research.