

1. Presenter: Pavani Cherukupally
Author(s): Pavani Cherukupally, Wei Sun, Daryl Williams, Geoffrey Ozin, Amy Bilton, and Chul Park
Title: Remediation of Oil Sands Tailings Using Green Nanoengineered Sponge

In Canada, over 5 million gallons of the oil contaminated water generated each day by steam-based oil extraction processes. One of the biggest challenges in treating these effluents is the removal of crude oil droplets due to its high salinity. Current materials, membranes and adsorbents are ineffective due to fouling, or slow response. Alternatively, sponges have micropores thus adsorb oil droplets effectively. This research focuses on the application of surface charge property required for usage of sponges as a filtration media. The oil field effluents are enriched with both positive and negative ions due to its high salt concentration. Thus, the oil droplets and the acid-base polymers attract ions but of opposite charge. This phenomenon results in attraction between the droplets and the sponges. In this work, an acid-base polymeric sponge was evaluated for its surface charge property to show its potential as a practical adsorbent. The sponge effectively adsorbed the crude oil droplets under various salt concentrations. As the salt concentration increased, the time of removal dramatically declined, resulting in over 99% of oil removal within 5 minutes. Also, in regeneration process, the crude oil was recovered from the sponge. In conclusion, the sponge was shown to be effective and reusable, resulting in recovered crude oil. Thus, the sponge filter has a great potential to be disruptive in remediation of oilfield effluents and generate value from otherwise unusable waste.

2. Presenter: Karl Z. Demmans
Author(s): Matthew V. Gradiski, Molly M.-H. Sung, Robert H. Morris
Title: Morris Group Iron Chemistry

Since a breakthrough in 2008 on the discovery of catalysts that utilize iron for the reduction of polar bonds, our lab has been focused on producing catalysts based on this benign metal that are complexed with organic compounds. These new iron compounds may replace industrial scale catalysts based on toxic, rare and expensive metals such as ruthenium, rhodium or palladium that are used in the pharmaceutical, fragrances and flavours industry. Our current generation of iron catalysts are extremely active, surpassing the activity of precious metal catalysts.

3. Presenter: Aseel Al Nimer
Author(s): Aseel Al Nimer
Title: Bulk and Surface Chemistry of Iron in the Formation and Aging of Secondary Organics Relevant to Atmospheric Systems

Atmospheric aerosols impact climate, human health and air quality through their direct and indirect effects. Secondary organic aerosols (SOAs) are generated when aliphatic and/or aromatic volatile compounds (VOCs) from natural and anthropogenic sources are oxidized in the atmosphere to form low-volatile products that undergo condensation on pre-existing particles. Transition metals, particularly iron (Fe) could significantly play a role in aging and formation of secondary organic aerosols through heterogenous/multiphase reactions. Moreover, abundant organic aerosols like oxalate an end product of photochemical oxidation of VOCs and inorganic aerosols like sulfate a product of gaseous phase oxidation of SO₂, could affect the role of iron in this formation and aging process. However, the knowledge regarding this role in term of bulk and surface chemistry of iron in multicomponent aerosol systems and in the presence of abundant organic and inorganic species such as oxalate and sulfate remains poor and needs more investigation. This poster will highlight the effect of oxalate and sulfate species on iron-catalyzed SOA formation reactions. In addition, this chemistry could predict the reactivity of other atmospherically relevant and iron-containing surfaces that include soil, oceans and built environments.

4. Presenter: Shegufa Shetranjiwalla
Author(s): Shegufa Shetranjiwalla and Andrew Vreugdenhil
Title: Waterborne epoxy-thiol decorated silica sol-gel coatings: Impact of crosslinking on corrosion prevention

Organic-inorganic hybrid coatings of crosslinked epoxy and thiol silicates (TGST) were synthesized for the corrosion protection of low carbon steel via a waterborne sol-gel route. The coatings were synthesized in two stages; in the first step two separate aqueous formulations of epoxy and thiol decorated silica colloids were prepared and subsequently crosslinked in a 1:1 ratio in the second stage. The structure and rate of crosslinking was monitored using Raman spectroscopy. Formulation stability was measured based on viscosity changes and pot-life assessment. The novel crosslinked material was characterized for its particle size using dynamic light scattering and viscosity average molecular weight was calculated using Fikentscher's equation and associated with polyethylene oxide molecular weights. The covalently bonded epoxy-thiol silicate coating was uniform, defect free. Accelerated corrosion resistance was tested by exposing the panels to standard salt solution tests. TGST showed a 96% improvement in corrosion inhibition over the non- crosslinked formulations in a corrosive environment. The synthesis and characterization of TGST using a simple approach, revealed key synthetic parameters for generating optimized sol-gel corrosion prevention materials.

5. Presenter: Shegufa Shetranjiwalla
Author(s): Shegufa Shetranjiwalla and Suresh S. Narine
Title: Entirely lipid-derived thermoplastic poly(ester urethane)s: Effect of structure on physical properties

Thermoplastic poly(ester urethane)s derived from vegetable oils possess inferior physical properties compared to their entirely petroleum-based counterparts due to structural limitations and lower reactivity of the precursor lipid-derived monomers. The present work shows that high molecular weight of TPEUs can be prepared from lipid-derived monomers via the synthesis of polyester diols with controlled molecular weights, tuning of the functional group stoichiometry of the polyester diols and the diisocyanate during polymerization, the degree of polymerization and control of the hard segment hydrogen bond density and distribution via the use of a chain extender and different polymerization protocols.

Solvent-resistant TPEUs with high molecular weight displaying polyethylene-like behavior and controlled polyester and urethane segment phase separation were obtained. Structure-property investigations revealed that thermal transition temperatures and tensile properties increased and eventually plateaued with increasing molecular weight. Novel segmented TPEU elastomers possessed high phase separation and were rubber-like with low modulus and high elongation. The response of the structurally optimized TPEUs to environmental degradation was also established by subjecting the elastomers to hydrothermal ageing.

TPEUs exhibited thermal and mechanical properties which were comparable to commercially available entirely petroleum-based analogues, and which could be tuned in order to achieve enhanced physical properties and controlled degradability.

6. Presenter: Mohammad Mahaninia
Author(s): Mohammad H. Mahaninia and Lee D. Wilson
Title: Cross-linked chitosan beads doped with calcium for organophosphate removal from aqueous solution

The organophosphates (OPs) are compounds that are widely used as pesticides. The use of OPs has increased the the level of phosphate species in aquatic environments. These compounds are listed as very highly acutely toxic chemicals for humans and environment and research concerning the effective removal of OPs removal has become an area of vital inquiry. In this research, chitosan beads were cross-linked with glutaraldehyde (GA) and epichlorohydrin (EP), respectively, at variable composition level followed by imbibing into solutions of calcium ions. Characterization of the prepared materials was investigated using various techniques to scrutinize the effect of modification on the structure and chemistry of chitosan. Adsorption properties of bead materials toward p-nitrophenyl phosphate (PNPP) was studied at pH 8.5 where isotherm results were analyzed using the Sips model. Cross-linked materials with glutaraldehyde demonstrated higher affinity toward PNPP. The calcium doping on the materials with lower cross-linking content resulted in an enhanced uptake toward PNPP.

7. Presenter: Darius Hung
Author(s): Darius Hung, Chenxi Qian, Wei Sun
Title: Catalytically Active Silicon Hydride Nanosheets for CO₂ Reduction

Heterogeneous conversion of CO₂ to value-added chemicals and fuels by Si surface hydrides has recently attracted broad research interest. Being earth abundant, low-cost and non-toxic, Si is one of the most promising candidates for comprising such a catalyst that can offer the solution to a future CO₂ conversion to synthetic fuels on the grand scale of giga tonne per year. However, the silicon hydrides are known to stoichiometrically react with CO₂ and attempts reported so far have all failed in the catalytic conversion of CO₂. The deactivation of Si originates from the formation of inactive surface silanols and siloxane groups and permanent loss of Si hydrides. Here, aiming at cracking the core of the problem, we deposited Pd nanoparticles on Si nanosheet surface using an innovative synthetic strategy. In situ infrared study showed that Si hydrides were successfully regenerated on such surfaces exposed to CO₂ and H₂. We demonstrate for the first time that 2D nanosheets of hydride-capped silicon decorated with Pd nanoparticles, in an unprecedented catalytic cycle, can enable the reverse water gas shift reaction, with a pronounced light effect.

8. Presenter: Yuchan Dong
Author(s): Yuchan Dong, Kulbir Kaur Ghuman, Radian Popescu, Paul N. Duchesne, Wenjie Zhou, etc.
Title: Tailoring Surface Frustrated Lewis Pairs of In₂O_{3-x}(OH)_y for Gas-Phase Heterogeneous Photocatalytic Reduction of CO₂

Frustrated Lewis Pairs (FLPs) created by sterically hindered Lewis acids and Lewis bases have shown their capacity for capturing and reacting with a variety of small molecules, including H₂ and CO₂, and thereby creating a new strategy for CO₂ reduction. In this work, the photocatalytic CO₂ reduction behavior of defect-laden indium oxide (In₂O_{3-x}(OH)_y) was greatly enhanced through isomorphous substitution of In³⁺ with Bi³⁺, providing fundamental insights into the catalytically active surface FLPs (i.e., In-OH...In) and the experimentally observed 'volcano' relationship between the CO production rate and Bi³⁺ substitution level. According to density functional theory calculations at the optimal Bi³⁺ substitution level, the 6s² electron pair of Bi³⁺ hybridizes with the oxygen in the neighboring In-OH Lewis base site, leading to mildly increased Lewis basicity without influencing the Lewis acidity of the nearby In Lewis acid site. Meanwhile, Bi³⁺ can act as an extra acid site, serving to maximize the heterolytic splitting of reactant H₂, and results in a more hydridic hydride for more efficient CO₂ reduction. This study demonstrates that isomorphous substitution can effectively optimize the reactivity of surface catalytic active sites in addition to influencing optoelectronic properties, affording a better understanding of the photocatalytic CO₂ reduction mechanism.

9. Presenter: Mireille Ghoussoub
Author(s): Lu Wang*, Mireille Ghoussoub*, Hong Wang, Yue Shao, Wei Sun, Athanasios A. Tountas, Thomas E. Wood, Hai Li, Joel Yi Yang Loh, Yuchan Dong, Meikun Xia, Young Li, Shenghua Wang, Jia Jia, Chenyue Qiu, Chenxi Qian, Nazir P. Kherani, Le He, Xiaohong Zhang, Geoffrey A. Ozin
Title: Photocatalytic Hydrogenation of Carbon Dioxide with High Selectivity to Methanol at Atmospheric Pressure

Abstract: The production of solar methanol, directly from gaseous CO₂ and H₂, is important for the development of a sustainable energy economy. Despite growing activity in the field, very few photocatalysts exist that can efficiently and stably hydrogenate gaseous CO₂ to methanol at ambient pressure with high selectivity. Here, we report that a defect-laden indium oxide, In₂O_{3-x}(OH)_y, with a rod-like nanocrystal superstructure, can photocatalyze the hydrogenation of CO₂ to methanol with 50% selectivity under simulated solar irradiation. Notably, the solar methanol production of the In₂O_{3-x}(OH)_y nanocrystal superstructures can be stabilized at a rate of 0.06 mmol g⁻¹ h⁻¹ at atmospheric pressure. This is 120 times higher than that of the best-known photocatalysts. This discovery bodes well for the development of a low-pressure solar methanol process using CO₂ and renewable H₂ feedstocks.

10. Presenter: Mohammad Aminur Rahman
Author(s): Arthur Situm, Hind A. Al-Abadleh
Title: ATR-FTIR Studies on the Initial Binding Kinetics of Arsenicals at the Organic-Hematite Interface

The environmental fate of arsenic compounds depends on their surface interactions with geosorbents that include clays, metal oxides and natural organic matter (NOM). Here, we report the adsorption kinetics of arsenate and dimethylarsinic acid (DMA) with hematite nanoparticles pre-exposed to three types of low molecular weight organics: citrate, oxalate and pyrocatechol as representatives to most reactive organic functional groups in NOM. These studies were conducted using attenuated total internal reflection Fourier transform infrared spectroscopy (ATR-FTIR) at pH 7 with an emphasis on the role that electrolytes (KCl, NaCl and KBr) play in the adsorption process. Results show that negatively charged carboxylate versus hydrophobic phenyl groups influence amounts and initial rates of arsenicals adsorption on hematite nanoparticles to varying degrees depending on the types of complexes they form. Secondly, the type of electrolytes affects initial adsorption rate of DMA to a greater extent than arsenate while oxalate is present on the surface. Thirdly, the extent of organics retention by hematite nanoparticles is influenced by the type of the designing agent. These results are significant considering the interactions of low molecular weight NOM and their effect on arsenicals binding to iron (oxyhydr)oxides that is ubiquitous in environment.

11. Presenter: James H. W. LaFortune
Author(s): James H. W. LaFortune, Julia M. Bayne, Louie Fan, and Douglas W. Stephan
Title: A Robust Lewis Acidic Phosphonium Catalyst in the Synthesis of Heterocycles via Hydroarylation of Alkynes

Our group has recently developed highly Lewis acidic phosphorus-based cations capable of catalyzing many reactions. By combining recent advancements in our lab, we have achieved an air and moisture stable phosphorus-based catalyst that maintains reactivity. In searching for new catalytic applications, we noted that strong Lewis acids mediate hydroamination with terminal alkynes and that, although our phosphorus-based cations have demonstrated hydroarylation with alkenes, the analogous alkyne reactivity has not been explored. This poster presents this robust phosphorus-based catalyst's reactivity with arylamines and alkynes to produce heterocyclic compounds.

12. Presenter: Thomas Wood
Author(s): Thomas Wood, Paul Duchesne, Thomas Dingle, Alexandra Travasoli, Mireille Ghossoub, Athan Tountas, Lourdes Hurtado, Yuchan Dong, Young Li, Navid Soheilnia, Geoffrey Ozin
Title: Solar Fuels - Next Gen Fuel from CO₂

Greenhouse gas emissions and dependence on fossil fuels are key challenges facing humanity in the 21st Century. The Solar Fuels Group, a semi-finalist of the Ontario 2030 Solutions challenge, is addressing these challenges by developing novel nanomaterials that can act as photocatalysts for the conversion of CO₂ into hydrocarbon fuels and chemical feedstocks. Sunlight powered conversion of carbon dioxide and water vapor to fuels holds out the promise of large-scale electrical generation fueled entirely by the energy of the sun. At the heart of this challenge lies the exceptionally high thermodynamic and kinetic stability of CO₂. In the case of solar fuels, this requires the discovery of highly active photocatalysts and the development of high performance photoreactors. To meaningfully impact climate change, targeted catalysts must be able to make synthetic fuels from CO₂ at industrially practical scales and rates of conversion, while maintaining long-term performance stability. In addition, the catalyst must comprise earth-abundant, low-cost, non-toxic elements, to ensure economically viable and environmentally sound CO₂ refineries. To actualize this utopian idea of a green and sustainable future, the Solar Fuels group is inventing nanostructured materials that can accomplish this conversion efficiently, safely, and economically on a large scale.

13. Presenter: Carson Chu

Author(s): Carson Chu, Prof. Murray J. Thomson

Title: The chemical structure effects of alkylbenzenes on soot formation in a laminar co-flow flame

The chemical structure effects of alkylbenzenes (1,2,4-trimethylbenzene (124TMB) and n-propylbenzene (PBZ)) on soot formation in a laminar diffusion flame were experimentally and numerically investigated in this study. In the experiment, the optical laser-induced incandescence (LII) and spectral soot emission (SSE) diagnostics were used to measure radial soot volume fraction, primary particle diameter and flame temperature profiles. The radial number density and centerline specific surface growth rates were also derived experimentally. The results are consistent with the literature as 124TMB exhibits higher soot concentration than PBZ. From the analyses of the derived number density and specific surface growth rates, this is caused by the higher soot nucleation rate for 124TMB. This conclusion is supported by the numerical modelling, which utilized the detailed CoFlame code with a moderately reduced Ranzi mechanism. The simulation results show that 124TMB has earlier soot inception and Polycyclic Aromatic Hydrocarbon (PAH) addition than PBZ. Consistent with both earlier soot inception and PAH addition, 124TMB also has earlier pyrene (A4) formation, suggesting 124TMB has alternative reaction pathways for pyrene formation. The reaction pathway analysis shows that pyrene is formed via the aromatic radical recombination route, as opposed to the conventional HACA mechanism. Bypassing the formation of the second ring is the reason for 124TMB having earlier soot nucleation. In contrast, the formation of pyrene for PBZ follows the slower HACA pathways, leading to later soot nucleation.

14. Presenter: Anton Sediako

Author(s): Anton Sediako, Murray J. Thomson

Title: In Situ Electron Microscopy Studies For Clean Combustion

Atmospheric soot, an undesired product of incomplete hydrocarbon combustion, has been found to be the most harmful air pollutant, penetrating deep into lung tissue, blood streams, and causing a host of health issues such as cancer and heart disease. Apart from health effects, it is also the second largest contributor to climate change, while also negatively affecting combustor and engine efficiencies. The present work aims to analyse and understand the effects such as combustor pressure, catalysts, and temperature on the nanostructure of soot, and its effect on oxidation by in situ experiments inside of an Environmental Transmission Electron Microscope (ETEM). The combination allows for the first time, a unique opportunity to observe the internal nanostructure of soot, and visualize the internal/surface oxidation, fragmentation, and structural changes. Such work allows for the design of cleaner combustors and novel catalysts.

15. Presenter: Kathleen Hefferon

Author(s): Kathleen Hefferon, Borja Cantero, Uzma Badar

Title: Production of A Universal Plant-Based Substrate System for Cellulase Activity Assays

Cellulases and other cell wall degrading enzymes are currently being engineered with improved traits for application in the breakdown of lignocellulosic biomass. The majority of assays with these 'designer' enzymes have been carried out using synthetic substrates such as crystalline bacterial microcellulose (BMCC). The use of synthetic substrates may not reflect the actual action of these cellulases on real plants. In the following study, suspension cell walls from several plant species were examined as possible alternatives for synthetic cellulose substrates.

16. Presenter: Spencer Imbrogno
Author(s): Spencer Imbrogno and Emma Master
Title: Chemo-Enzymatic Upgrading of Hemicellulose Oligosaccharides

Most recent applications of enzymes for carbohydrate processing have concentrated on the conversion of polysaccharides (e.g. cellulose) to monosaccharides (e.g. glucose) for conversion to fuels and platform chemicals by fermentation or chemical routes. Alternatively, enzyme selectivity can be utilized to introduce new functionality to enhance the reactivity and promote the reassembly of hemicellulose fractions to produce bifunctional building blocks. This approach has been demonstrated using acidic hemicellulose oligosaccharides to prepare bio-based polymers. It is hypothesized that enzyme selectivity can be harnessed to prepare hemicellulose based aldehyde crosslinking molecules for wood adhesive applications or to enhance the properties of bio-based materials such as films or gels. These aldehyde crosslinkers could be used as replacements for toxic, petrochemical based aldehydes such as glyoxal and formaldehyde used in wood composites and other products. The chemoenzymatic pathway to prepare aldehyde crosslinkers was demonstrated using lactose as a hemicellulose model. Enzymes glucooligosaccharide oxidase and galactose oxidase were used to introduce new functional groups that allowed coupling with amines and subsequent formation of aldehyde-containing crosslinking molecules. These aldehyde-containing molecules were then used to crosslink and modify the properties of polyols. Further work will investigate the properties of the crosslinked materials and the ability to tailor the properties of the crosslinking molecule based on amine selection. Ideally bio-based amines such as peptides can be utilized and their properties can be controlled in order to enhance the performance of the crosslinkers.

17. Presenter: Sara Soldoozy
Author(s): Sara Soldoozy and Dr. Hind Al-Abadleh
Title: Using ATR-FTIR Spectroscopy for Determining Activation Energy of Adsorption on Hematite Nanoarticles

Iron-containing materials have a great affinity to arsenical compounds. For the purpose of water treatment and arsenic removal from contaminated water, hematite nanoparticles or Fe-(oxyhydr) oxide are considered effective materials. In this research, the activation barrier for the adsorption of dimethylarsinic acid (DMA) from solution to hematite nanoparticles was extracted. Spectra were collected using attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) as a function of time, concentration and temperature (5-50C) at pH 7. This technique is best suited for the in-situ surface complexation studies. The Langmuir adsorption model was used to fit the kinetic curves and obtain rate parameters. Activation energy (E_a) was calculated using the Arrhenius equation. This study is significant because it will highlight how organic substitution on arsenate affects adsorption rates and hence strength of binding to arsenic removal media.

18. Presenter: Maryam Arefmanesh
Author(s): Maryam Arefmanesh, Emma R. Master, Mojgan Nejad
Title: Lignin modification for Bio-based resin application

Abstract: Lignin is the most abundant natural polyaromatic plant-derived macromolecule in the world. Majority of lignin is currently used by pulp and paper mills as a source of energy, whereas the presence of aliphatic and aromatic hydroxyl groups in lignin structures makes it a good candidate for higher-value applications, including alternatives to replace petroleum-derived polyols (e.g., polyether polyol and phenol formaldehyde) used for polyurethane resin (PU) and PF formulation. The aim of this study is to establish a sustainable pathway to increase the reactivity of lignin suitable for application in resin formulations. In addition to comparative analyses using at least four lignin samples from different isolation methods and resources (e.g., lignin recovered from kraft, organosolv, and steam explosion/enzymatic hydrolysis processing of wood or agricultural sources), the potential of ionic liquids (ILs) and enzymes to increase the hydroxyl content of lignin samples (i.e., more than 30%) will also be investigated.