ACS
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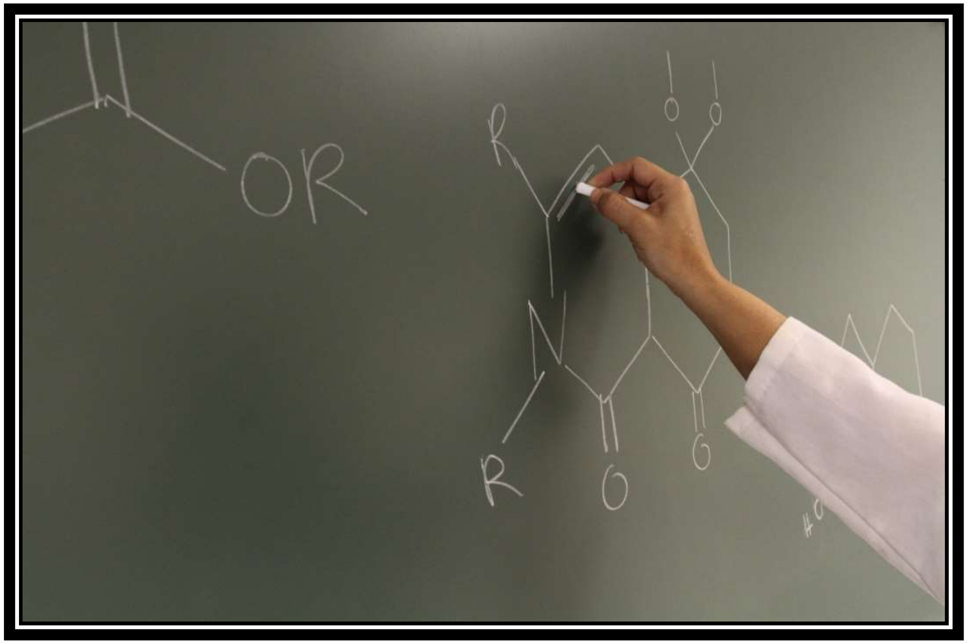
Indiana Section
American Chemical Society

“Think Like a Molecule”

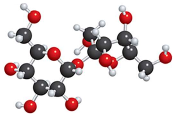
2019 Poster Session



April 5, 2019

IUPUI Science & Engineering Laboratory Building
350 N Blackford St., Indianapolis, IN 46202

Sponsored by the
American Chemical Society, Indiana Section
and IUPUI School of Science



science@iupui

Keynote Speaker: Matthew M. Gardlik, Ph.D.

Patent and Trademark Attorney

Matt is an avid technologist and his interests range from computer programming to organic synthesis. As an undergraduate, Matt received Wittenberg University's Division of Analytical Chemistry Award for construction and programming of a computer-controlled automatic titrator. As part of this award, he became a member of the American Chemical Society (ACS) in 2001.

He earned his Ph.D. at The Ohio State University where his dissertation involved organic synthesis and supramolecular chemistry. He developed an optimized synthetic route to a key intermediate in the synthesis of a new class of supramolecular hosts called "molecular baskets." This work enabled the scale-up and preparation of several hosts that was critical for studying their encapsulation properties.

Matt continues to be involved in the ACS and was awarded the 2012 Catalyst Award by the Cincinnati Section of the ACS for his contribution to the Local Section. In November 2013, he was elected Chair of the Indiana Section of the ACS. He helped to organize the national ACS meeting in 2013 which was held in Indianapolis and has served as webmaster and election chair for several years.

Matt is currently a patent and trademark attorney and Partner at Woodard, Emhardt, Henry, Reeves & Wagner LLP (uspatent.com) in Indianapolis, Indiana where he has worked since graduating from law school in 2012.

Matt's practice includes the preparation and prosecution of patent applications as well as assisting in the firm's litigation cases. Matt has been involved in litigation where the damages sought are several hundred million dollars. For example, Matt was a key member of a litigation team which successfully defended an accusation of trade secret misappropriation where the plaintiff was seeking over $200MM. After a two-week jury trial, the jury found that the plaintiff failed to prove existence of the trade secret. Matt is also the sole chemist and key team member and strategist in a patent infringement litigation regarding polymer binder chemistry where our team represents the patent owner and plaintiff. This litigation involves nine asserted patents, and our team successfully defended these patents in 13 Inter Partes Review proceedings at the patent office.

While assisting with litigation matters, Matt continue to be extensively involved and enjoys all aspects of patent prosecution including preparation and prosecution in the chemical, pharmaceutical, diagnostic, and medical device arts. Matt's prosecution experience not only includes practice with the USPTO, but also directing the work of foreign associates in patent offices around the world. Matt frequently assist in representation of a large privately-held medical device manufacturer in Indiana.

Poster Session Awards

2019 ACS Poster Session Winner (All Posters Eligible)
- Grand Prize Winner
- $500 prize, Plaque Award and Certificate

ACS Project SEED Award (High School Posters Only)
- 1 Winner only
- $100 prize, Plaque Award and Certificate

Kurek Student Award (Undergraduate Posters Only)
- 1st Place; $100 prize, Plaque Award and Certificate
- 2nd Place; $50 prize and Certificate
- 3rd Place; $25 prize and Certificate
- Honorable Mention: Certificate

ACS Chair’s Award (All Posters Eligible)
- 1st Place; $100 prize, Plaque Award and Certificate
- 2nd Place; $50 prize and Certificate
- 3rd Place; $25 prize and Certificate
- Honorable Mention: Certificate

IUPUI Dean’s Award (All Posters Eligible)
- 1st Place; $100 prize and Plaque Award and Certificate
- 2nd Place; $50 prize and Certificate
- 3rd Place; $25 prize and Certificate
- Honorable Mention: Certificate

ACS POSTER SESSION

Event schedule

4:00 pm – 5:00 pm
Poster presenters check-in and set up poster

5:10 pm – 6:10 pm Session 1 (odd)
6:15 pm – 7:15 pm Session 2 (even)
Poster session and reception

7:20 pm – 8:00 pm
Keynote address – Matthew Gardlik, Ph.D.
Patent Lawyer for Woodard, Emhardt, Henry, Reeves, & Wagner, LLP

8:00 pm – 9:00 pm
Presentation of awards

April 5, 2019

Dear Participants & Guests,

Welcome to our “Think Like a Molecule” Poster Session! That’s what a popular chemistry professor, Joseph T. Kurek, encouraged all around him to do. Joe received his PhD at Purdue University under Herbert C. Brown, who won the Nobel Prize in Chemistry laureate for his work with organoboranes. He taught chemistry for many years at Franklin College and was an adjunct professor at UIndy prior to joining Heritage Research Group (HRG). His influence was remarkable until his last breath.

Representing the Indiana Section of the ACS, we extend a special thanks to IUPUI for hosting this event. Simon J. Rhodes, Ph.D., Dean of the School of Science at IUPUI, has been an avid partner with the Indiana local section of the American Chemical Society for which we are extremely grateful. Tamiko Porter, chemistry lecturer at IUPUI and Chair of the Organizing Committee has been instrumental in making this happen.

Fourteen awards will be presented this evening to the top posters.

- Grand Prize ACS Poster Award Winner
- IUPUI’s Dean's Poster Presentation Award
    - First, Second, Third Place & Honorable Mention
- ACS Chair's Poster Presentation Award
    - First, Second, Third Place & Honorable Mention
- Kurek Student Poster Presentation Award
    - First, Second, Third Place & Honorable Mention
- Project Seed Poster Award

Thank you for participating in this poster session. We hope that you enjoy the networking opportunities and learn from other researchers. We hope you always enjoy thinking like a molecule!

Best wishes,

The Indiana Local Section of the American Chemical Society

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Next ACS National Meeting

Chemistry & Water
Fall 2019
August 25 - 29
San Diego, CA

* * *

- Fill out an evaluation
- Get a raffle ticket to win one of the following prizes:

prizes!

Apple iPad ~ Bluetooth Earbuds Wireless Headphones ~ Periodic Table Soft Fleece Throw Blanket

ACS Organizing Committee

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Your ACS local section is getting ready for:

If you are interesting in participating in the preparation for this 2023 meeting, please contact Frederique Deiss: fdeiss@iupui.edu

Indiana Section
American Chemical Society

2019 ACS Indiana Section Upcoming Events

Event	Date	Location
Science Day at Ball State	4/14/2019	Ball Gym
Earth Day	4/22/2019	Military Park
Awards night	5/22/2019	UIndy
Baseball Night	July - TBD	Victory Field
Fall National ACS Meeting & Exp.	Aug 25-29	San Diego, CA
Celebrate Science Indiana	10/5/2019	Indiana State Fairgrounds
NCW – Chemistry Day	11/3/2019	Children's Museum
Indiana Bicentennial - Frederique	April 3,4 -2020	Indiana Convention Center

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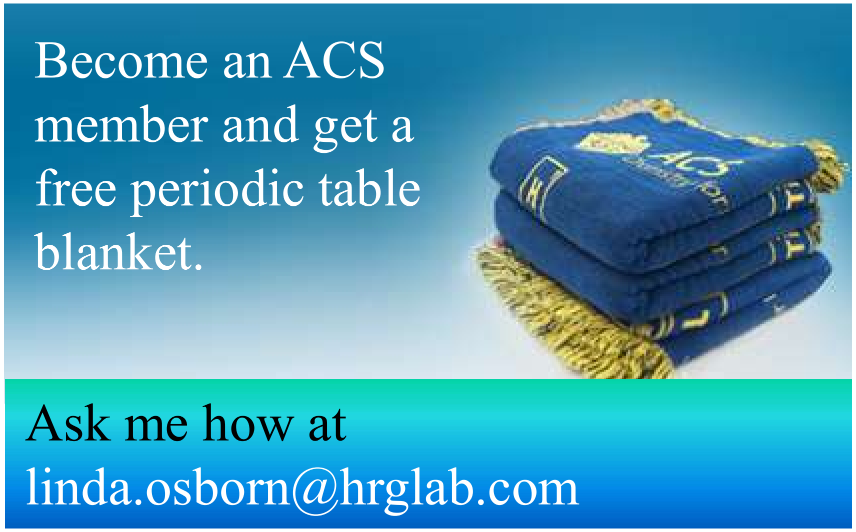
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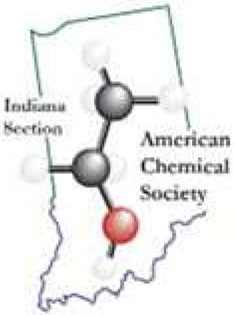
VISION

Our vision is to engage our members and community to advance the broader chemistry enterprise for the benefit of Indiana and beyond.



MISSION

It is the Mission of the Indiana Local Section of the American Chemical Society to improve people's lives through the transforming power of chemistry.

http://www.acsindiana.org/acs/

Poster 1.

Authors: Paula Andrea Angarita Rivera, Mangilal Agarwal, Amanda Siegel, Meghana Teli, Ali Daneshkhah, Mark Woollam and Hiroki Yokota

Title: Comparing Untargeted Metabolomic VOC Analyses on Different Gas Chromatography Mass Analyzers: Single Quadrupole (MS) vs Quadrupole Time-of-Flight (QTOF)

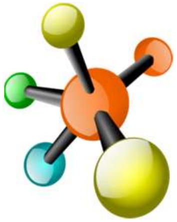
One in eight women will likely test positive for breast cancer in their lifetime. For this reason, it is important to diagnose potential patients before cancer metastasizes. Screening test are the primary method used by physicians to detect breast cancer in patients before a biopsy is performed. However, from the biopsy only 20% of those patients have breast cancer. The current screening method is not very efficient and there is no other method that accurately determines if a patient has breast cancer or not. Volatile organic compounds (VOCs) are metabolites that can serve as biomarkers for different types of diseases. An effective method to analyze these VOCs is using gas chromatography-mass spectrometry. There are two common types of mass analyzers which differentiate ions by their mass to charge ratio (m/z): single-quadrupole (GC-MS) and quadrupole time-of-flight (GC-QTOF). The goal is to demonstrate that these mass analyzers can identify the same statistically significant biomarkers that can distinguish between localized and delocalized breast cancer. A total of 18 mouse urine samples were analyzed by using both instruments. Eight urine samples were collected from mice with cancer in the mammary pad and ten from mice with cancer metastasized to the bone. Multivariate analysis such as Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA) and Leave One Out Cross Validation (LOOCV) were used to identify the statistically significant biomarkers present in breast cancer. The results demonstrate that a total of 7 biomarkers are present in both data sets (95% accuracy). Furthermore, these biomarkers, if confirmed in human studies, could be used to design a resistive based sensor to detected breast cancer non-invasively in human urine.

Poster 2.

Authors: Kymeri Davis and John Goodpaster

Title: An Overview of Total Vaporization Solid Phase Microextraction (TV-SPME) and its Forensic Applications

While Gas Chromatography – Mass Spectrometry (GC-MS) is a frequently used technique in forensic science laboratories, there are limitations such as the need for compounds to be thermally stable as well as volatile. Some compounds must undergo derivatization prior to being injected into the gas chromatograph (GC) to satisfy these requirements. Solid-Phase Microextraction (SPME) is a technique in which analytes are absorbed onto a fiber which is then placed inside the GC inlet for desorption. Total Vaporization-SPME (TV-SPME) utilizes the same technique as standard SPME but vaporizes a sample extract that is then absorbed onto the fiber. On fiber derivatization may also be performed using TV-SPME. The polydimethylsiloxane-divinylbenzene (PDMS-DVB) fiber is first exposed to a vial containing the derivatization agent. The SPME fiber is then exposed to a new vial containing the analyte of interest. TV-SPME is beneficial because it allows for the analyte to be derivatized during the extraction process which reduces analysis time. TV-SPME may be used to analyze drugs and drug metabolites in urine and beverages and may also be used in the analyses of fuel samples and explosive compounds. There are currently numerous methods and techniques available for the analysis of controlled substances, however, these methods often require sample preparation such as an extraction. This TV-SPME method requires little to no sample preparation and utilizes a simple GC-MS method.



Poster 3.

Authors: Brittany Rauzan, Dennis Wujek and John Atkinson

Title: Development of Crop Protection Products for Sustainable Agriculture

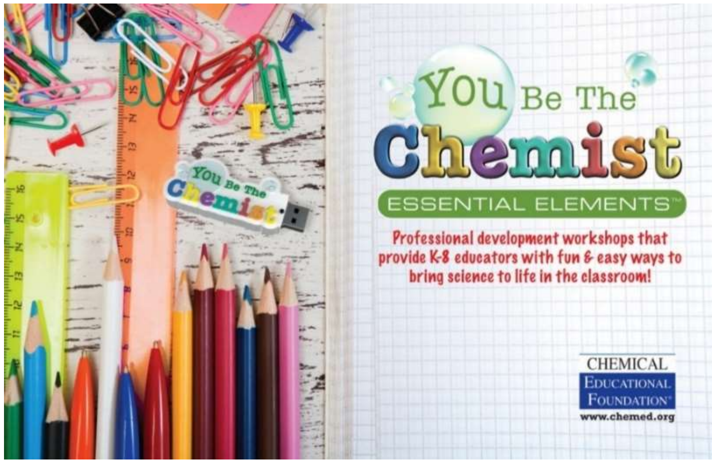
Green Chemistry principles are crucial in agriculture due to the sheer size of the food value chain. At Corteva Agriscience™, we are developing innovative, sustainable solutions to increase food production for the rapidly expanding global population. In this presentation, we will highlight several examples applying sustainability principles to formulation development for crop protection products that meet the needs of farmers and consumers, while minimizing the ecological footprint.

Poster 4.

Author: Kelsi Goshinsky, Zhihai Li and Cody Leasor

Title: Characterization of Nanomaterials and Solar Cell Electrodes by Atomic Force Microscopy

As one of the most powerful tools in nanoscience and nanotechnology, atomic force microscopy (AFM) has been widely used in many fields including biology, chemistry, physics and materials. In this poster, we first introduce AFM principle, i.e., how AFM can image surface morphology, and continue to describe the procedure of how to carry out an AFM experiment in our lab. Then, we will present some experimental data on the characterization of different nanomaterials (such as $NiWO4$, $TiO2$) and solar cell electrodes using taping mode AFM imaging technique. The high-resolution AFM images show that morphology and size of $NiWO4$ nanomaterials can be determined. AFM images also reveal different surface morphology before and after depositing $TiO2$ and platinum nanomaterials on solar cell electrode surface.



National Chemistry Week 20 Years

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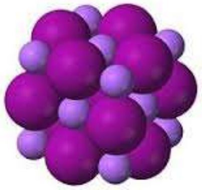
Poster 5.

Authors: Sydney Reynolds and Katherine Stickney

Title: Comparison of Name Brand Vs. Replicated Fragrances by GC-MS Analysis of Fragrance Components Volatilized from a Model Skin Surface

The following honors project involves the comparison of name-brand perfumes that are in high demand in the perfume market to more affordable perfumes that are known to have similar scents. Three name-brand/knockoff pairs were analyzed. The high-end fragrances that were studied include Chanel Coco Mademoiselle, Ralph by Ralph Lauren, and Viva la Juicy by Juicy Couture. These were compared to the cost-effective replicates Suddenly by Madame Glamour, Paris Hilton by Paris Hilton, and Siren by Paris Hilton, respectively. Perfumes are a complex mixture of fragment compounds, so this analysis was done using an Agilent gas chromatograph equipped with a mass spectrometer (a technique commonly referred to as GC-MS), which separates the compounds as they volatilize and identifies them by mass spectrometry. Each perfume was placed on a model skin surface and sealed into a gas-tight vial before sampling, to determine the selective adsorption/volatilization of the various perfume components, and the chemical profile of the gaseous phase of each name brane perfume will be compared to that of its knock-off. The profile of these samples was also compared to volatile components of a “blank” sample which consisted of perfume placed directly in a vial without the model skin surface. The goal of this study was to determine if the chemical composition and selective volatilization of the pairs of name-brand/knockoff perfumes are qualitatively similar or different.



Poster 6.

Authors: Princess Walker and Cori Jenkins

Title: Utilizing Dynamic Bonds to Modify Polysulfide

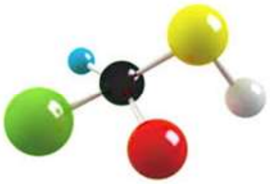
Inverse Vulcanization was created by Jeffrey Pyun et al as a way of utilizing the abundance of elemental sulfur and reacting it with another monomer. 60 million tons of elemental sulfur is produced from crude oil in the petroleum refinery process. The ability to modify polysulfides is a possible means to broaden the versatility of sulfur-based polymers. Utilizing the inverse-vulcanization method a 30:70 sulfur: divinylbenzene (DVB) poly(S-DVB) is created on a 5 g scale at 185 °C for 1 hour. Next, maleimide is grafted onto poly(S-DVB). This reaction occurs at 100 °C at varied time trials ranging from 15 min to 48 hours. The reaction occurs at 100°C because of the free radicals on the poly(S-DVB) will cleave allowing the maleimide to incorporate into the prepolymer. To aid miscibility between maleimide and poly(S-DVB), dimethylformamide was added to the reaction. As an effort to make this reaction solvent free we created a terpolymer by adding styrene to the poly(S-DVB) on a 30:35:35 ratios of sulfur-styrene-divinylbenzene. After completing the reaction, gel permeation chromatography (GPC) and nuclear magnetic resonance (NMR) are used to characterize the resulting polymer, poly(S-DVB-maleimide). The NMR spectra revealed that as the reaction time increases, more maleimide is incorporated. The molecular weight of poly(S-DVB) samples determined by GPC both before and after modification. Examining changes in the molecular weight revealed a substantial drop in the molecular weight after 24 hours indicating that the backbone of the poly(S-DVB) is still intact as the maleimide is incorporating into the structure until after 24 hours. Overall, we were able to create a graft polymer by utilizing the inverse vulcanization method to create a prepolymer and then using the prepolymer to create a graft polymer by reacting maleimide with poly(S-DVB) and DMF; while keeping the poly (S-DVB) backbone intact for at least 24 hours.

Poster 7.

Authors: Brandon Bills and Nicholas Manicke

Title: Concentrating and preserving THC and designer drugs through paper modifications for paper spray mass spectrometry

Overdoses on designer drugs has become a significant public health issue in recent years. Sample preparation and chromatography techniques add analysis time and cost to each sample and require training to perform. A fast, cheap and simple method for analysis is needed to help deal with the current crisis. Paper spray is a rapid ambient ionization technique in which a biofluid is spotted and analyzed directly from paper with a macroscopic point without further sample preparation. However, detection limits for these compounds, which are typically in the 1-10 ng/mL range, are too high to detect toxic levels in some cases. Using strips of paper, both by itself and with treatments, was investigated as a simple means to concentrate analytes out of biological matrices. Urine containing analytes of interest, such as fentanyl analogues, synthetic cannabinoids, and THC and its metabolites, were spotted at one end of a strip of paper. After the sample wicked to the other end of the paper the strip was cut into 5 mm increments and analyzed to determine which analytes concentrated in the first few mm of the paper and which evenly distributed. Sesame seed oil was investigated as a means of concentrating and preserving THC and its metabolites which are labile and difficult to analyze in dried spots. Finally, a cartridge compatible with an autosampler and capable of performing a paper strip extraction within the cartridge was designed and 3D printed. It was found that detection limits for THC, its metabolites and synthetic cannabinoids could be noticeably improved using paper strip extraction. In addition, adding sesame seed oil to the extraction end of the strip allowed for significantly improved detection limits after 27 days of storage at room temperature.

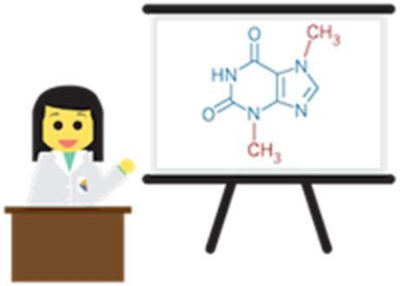


Poster 8.

Authors: Albert Mang

Title: Sost Genetic Deletion Modulates sFRP4 Effect on Bone Mass

Low bone mass due to aging or disability has significant financial and quality of life impact on our society. The search for therapies and treatments for skeletal fragility has many challenges, including off-target effects of certain compounds and a general lack of mechanistic understanding of basic cell biology. Naturally occurring genetic mutations in humans and other vertebrates can provide clues to implicate particular proteins as good drug targets. Such is the case with the two human diseases sclerosteosis (loss-of-function mutations in the SOST gene) and Pyle's disease (loss-of-function in the sFRP4 gene). Both of these mutations affect the WNT signaling pathway by reducing the pool of secreted WNT inhibitors. However, the two diseases have somewhat different and interesting phenotypes. Whereas SOST mutations result in increased bone mass across the skeleton (cortical and trabecular bone), sFRP4 mutations result in increased trabecular bone but reduced cortical bone mass. To determine whether the low cortical bone mass phenotype of sFRP4 deficiency could be rescued by deleting SOST, we bred sFRP4-null mice (sFRP4-/-) with Sost-null (SOST-/-) mice and quantified the skeletal phenotype radio graphically, using dual energy x-ray absorptiometry and micro CT. Bone mineral density was different in the different genetic models, especially between double knockouts and sFrp4 knockouts. Micro CT measurements, which can separate the cortical from cancellous contribution to bone mass, are underway. We hope to determine whether mutations that cause high cortical bone mass can rescue the low cortical bone mass phenotype of mice with mutated sFrp4.



Poster 9.

Authors: Sara Dille and Partha Basu

Title: The Effects Ligand Oxidation State Plays On Structure, Electronic, and Reactivity Properties of DMSO Reductase Mimics

Mononuclear molybdopterin enzymes are a large class of enzymes that are present in all phyla of life. All pterin containing enzymes posses a molybdopterin cofactor made up of a molybdenum metal center coordinated directly by a dithiolene ligand, which is appended to a pyranopterin cofactor. The majority of these enzymes catalyze oxygen atom transfer reactions that are concomitant with a transfer of two-electrons. We are hypothesizing that by altering the oxidation states of the dithiolene, the reactivity of the cofactor can be tuned for different substrates. This investigation focuses on the synthesis and characterization of oxo-MoIV(dithiolene) complexes that posses a fully reduced dithiolene ligand (dithiolene) and a fully oxidized dithiolene ligand (dithione). These complexes are designed to represent the asymmetry of the dithiolene ligand that is observed in the crystal structures of the DMSO reductase family. Dithiols such as benzene-1,2-dithiol, toluene-3,4-dithiol, quinoxaline-2,3-dithiol, and 3-6-dichloro-1,2-benzenedithol will represent the fully reduced dithiolene ligand. The asymmetric oxo-MoIV(dithiolene) complexes exhibit a unique structural property, a large fold angle along the S…S vector of the dithione ligand. These complexes also show a positive solvatochromic effect in a range of polar to nonpolar solvents. The rich electrochemical properties of these redox active complexes and other characterization details such as IR, and NMR studies will be presented. Effects on the reactivity of these complexes using biologically relevant substrates will be discussed. The oxygen atom transfer reactivity has been probed by mass spectrometry and NMR spectroscopy. The presented complexes aide in highlighting the effect redox state of the dithiolene ligand has in modulating reactivity.

Poster 10.

Authors: Breeanna Mintmier, Jennifer McGarry and Partha Basu

Title: Exchanging Protein Ligands to Examine the Impact of Molybdenum Coordination in Periplasmic Nitrate Reductase from Campylobacter jejuni

Periplasmic nitrate reductase (Nap), a molybdenum (Mo) enzyme, catalyzes the reduction of nitrate (NO3-) to nitrite (NO2-) in the periplasm, and yet the physiological role of Nap is not completely clear. It has been suggested that nitrate reduction may be involved in redox homeostasis, nitrate scavenging, nitrate respiration, and perhaps in pathogenicity. We present for the first time the heterologous overexpression of NapA from a pathogenic organism, Campylobacter jejuni. NapA, contains a molybdopterin cofactor where Mo is coordinated by two pyranopterin molecules and a cysteine residue. We hypothesize nitrate binds tightly to the Mo center of C. jejuni NapA due to the physiologically low nitrate concentrations found in the gut where C. jejuni colonizes. There are over 50 known molybdopterin enzymes with similar molybdenum cofactors yet they have different specificities for substrates and catalyze diverse reactions. Molybdopterin enzymes vary in the first coordination sphere of the Mo active site specifically the Mo coordinating residue. The coordinating residue has been hypothesized to tune the redox potential shifting substrate preference. For example, DMSO reductase that reduces DMSO to DMS and TMAO reductase that reduces TMAO to TMA have molybdenum centers coordinated by serine instead of cysteine. In order to study the tuning properties of the coordinating residue, recombinant native NapA and coordinating residue variants of NapA have been expressed. The kinetic properties of the native enzyme and the coordinating residue variants will be explored.

Poster 11.

Authors: Nikki Dodd

Title: Effects of mechanical stimulation on tumor growth and bone degradation in a mouse model of mammary tumor

In the United States, over 40,000 women annually lose their fight against breast cancer. Bone metastasis is a cause for a vast majority of these outcome. From previous studies, we have learned that in osteoporosis patients, weight-bearing activity such as jogging is considered to reduce bone degradation. It is unclear if the same type of mechanical stimulation may affect bone cells within breast cancer patients. We developed an in vivo model to evaluate the effects of axial bone loading following intra-tibial injections of cell line, 4T1.2 metastatic mammary tumor cells, into 17 BALB/c mice. We employed nine mechanically stimulated mice with 8 sham-loaded mice. Following the intra-tibial injections, we conducted a series of daily mechanical stimulation trials. Once completing the trials and sacrificing the mice, we conducted microCT and x-ray imaging of the tibiae. Our results reveal that in mice that experienced axial loading, greater bone degradation was observed than the sham loaded mice. The result demonstrates that mechanical loading could stimulate bone degradation. This may inform treatment of future breast cancer patients, but requires further investigation to analyze various factors in response to mechanical stimulation in the bone microenvironment.

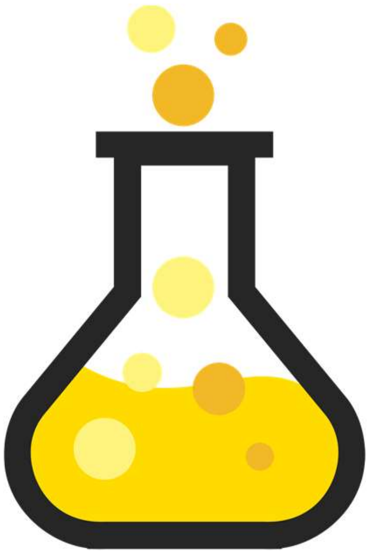
Save The Date!
Think Like a Molecule 2020
April 3-4, 2020
Beyond Boundaries: Indiana Academies Symposium

Poster 12.

Authors: Yifei Chen, Tykhon Zubkov and Zhihai Li

Title: Electrochemical Quantized Charging of Alkanethiol-Protected Gold Nanoparticles

Hexanethiol–gold nanoparticles are synthesized via the modified Brust-Schiffrin method, and characterized with TEM and scanning tunneling microscopy (STM) to discover the effect of ligand-to-gold molar ratio on the particle size. We have systematically varied the molar ratio of gold to protecting agent to discover the effect of gold-to-ligand ratio on the size of gold clusters. It is found that the average particle size decreases from 4.28 ± 0.83 nm to 1.54 ± 0.67 nm as the gold-to-ligand molar ratio changes from 1:1 to 1:9. When the ligand-to-gold ratio become small, gold atoms tend to form larger particles, and eventually make it impossible to form "nanoscale" particles when ligand-to-gold ratio is lower than 33% mole ratio (gold:thiol is equal to 3:1). Further, we also explored the electrochemical application of synthesize nanoclusters in terms of quantized charge at electrode-electrolyte interfaces, and capacitance of monolayer-protected nanoclusters were calculated.



Poster 13.

Authors: Mark Woollam, Amanda Siegel, Thomas Gardner, Imtiaz Munshi and Mangilal Agarwal

Title: Analyzing Urinary Volatile Metabolites to Develop a More Accurate Screening Method to Detect Prostate Cancer

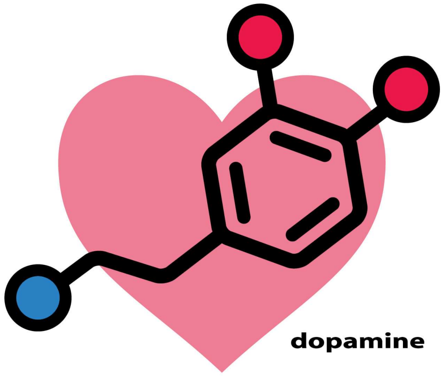
Prostate cancer is the second most common cancer in men with approximately 170,000 new cases diagnosed each year. The prostate specific antigen (PSA) test is the current screening method implemented to detect prostate cancer, but often produces inaccurate results. Urinary volatile organic compounds (VOCs) are end products of metabolism and may be a source of biomarkers for prostate cancer. Urine samples were collected and centrifuged, with the supernatant aliquoted into 10 mL headspace vials. NaCl was added to saturate the solution thirty minutes prior to GC-MS to concentrate volatiles in sample headspace. Samples were agitated at 60 °C for to drive volatiles into the headspace of the sample. VOCs were analyzed by solid phase microextraction (SPME) coupled to gas chromatography-mass spectrometry quadrupole time-of-flight (Agilent 7890A/7200) utilizing an automated PAL autosampler (CTC Analytics). 43 samples have been collected and analyzed so far from patients undergoing biopsy for prostate cancer. Data pre-processing procedures (Agilent Profinder) showed 504 features existing in at least 50% of one sample class. Univariate statistical analysis showed 27 features present with $p < 0.05$ that were up and down regulated in the prostate cancer sample class. Principal Component Analysis (PCA) showed promising separation between classes displaying the potential of metabolic VOCs to serve as biomarkers for prostate cancer.

Poster 14.

Authors: John Brown and Sergiy Rosokha

Title: Characteristics of Long Distance π Bonding Between Cation Radicals

Intermolecular π-bonding between ion-radicals is known as a critical factor in conductance and magnetic properties of organic materials and driving force for functioning of molecular machines. Yet, quantitative characteristics of strength of such long-distance bonding are lacking and the role of environment in these interactions is a subject of continuing debates. We addressed these problems via characterization of formation of π-bonded dimers between organic cation radicals. This was done by measurements of UV-Vis spectral changes in solutions of such radicals at various temperatures. These measurements showed conversion of absorption bands of monomers into that of dimers with decrease of temperature. Quantitative treatment of the UV-Vis spectral data afforded thermodynamic characteristics of π-bonding. Importantly, the use of bulky, weakly – coordinating anions minimized inter-ionic interactions. Preparation of single-crystals of the cation-radical salts and their X-ray crystallographic analysis provided structural characteristics of π-bonded intermolecular associates.



Poster 15.

Authors: Alexander Gordon, Birapar Singh, Alison Mertz, Arnize Ekwealor, Cullen Shorey, Ajay Panuganti, Asimiyu Tiamiyu and Jing Zhang

Title: 3D printing ceramic using a zirconium - silicate based ceramic slurry

Additive manufacturing (AM), also known as 3D printing, is a very useful technology for rapidly prototyping and experimenting with mechanical parts due to its ability to create custom shapes without having to create an expensive mold for material injection molding. Usually, AM uses plastic or metal as a material, however ceramic is more effective as a bio-compatible material. Ceramics tend to have very high compression strength and are very good insulators for electricity and heat. The ceramic we are using, zirconium silicate (ZS), is very useful for bio-medical devices and medical implants inside the human body. Zirconia, a similar ceramic does not have any adverse reactions in hard or soft tissue and even promotes bone growth when implanted in hard tissue. The ability to 3D print biomedical devices made of ZS would be advantageous because it could be custom made for a patient. ZS based ceramic also has the ability to store CO_2 and could potentially be used to capture CO_2 released from industrial machines. Proper layering of the zirconium silicate based ceramic is the primary focus for the research project. The ceramic will be 3D printed using a custom printer made in a previous project and then sintered inside an electric oven. The sintered and unsintered printed ceramic will be measured with a micro Vickers hardness tester to determine their hardness value (HV)and their surface structure.

Poster 16.

Authors: Azam Shafieenezhad, Horia Petrache and Bruce Ray

Title: Measurement of lipid vesicle charge in solutions of zwitterions

Binding of water soluble molecules to biological membranes is an important step in cellular signaling. We investigate the physical nature of such interactions using model lipid membranes. In particular, neutral lipid vesicles can acquire electrostatic charge by binding free ions from solution. Interestingly, they can also acquire charge from zwitterionic molecules that have dipole character. Examples are amino acids, pH buffers such as MOPS and HEPES, as well as adenosine triphosphate (ATP) and its hydrolysis products. By using x-ray scattering we have determined that the presence of zwitterions affects the lattice spacing of multilamellar phosphatidylcholine vesicles in a manner that is consistent with the presence of electrostatic repulsion between neighboring membranes. The remaining question is how to quantify the surface electric charge and, equally interesting, how to determine the sign of the charge conferred by zwitterions on membranes. Here we report measurements by dynamic light scattering (DLS) of phosphatidylcholine lipid vesicles in constant electric fields for a class of zwitterionic solutes. We find that the measured electrostatic charging can qualitatively account for the swelling of multilamellar structures and is consistent with NMR measurements of molecular binding. However, the results also show that more theoretical work is needed for quantitative analysis of electrostatic and van der Waals forces in these systems and for explanation of zwitterion affinities to biological membranes.

Poster 17.

Authors: John Peoples, Stephen Wassall and Andres Cavazos

Title: The Effect of Lipid Structure on Membrane Domain Formation

The coexistence of liquid-disordered (ld) and liquid-ordered (lo) phases in the phospholipid bilayer of cell membranes is believed to play a role in regulating cellular processes. How polyunsaturated fatty acid (PUFA)-containing phospholipids affect this fluid-fluid phase coexistence is proposed to contribute to the numerous health benefits associated with dietary intake of PUFA in fish oils. Our aim is to develop a method to study this behavior. Ternary mixtures of 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC, a PUFA-like lipid), 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC, a saturated lipid) and cholesterol (2:2:1) were prepared. Solid State 2H NMR spectroscopy of a deuterium labeled analog of DPPC (DPPC-d62) was used as a non-invasive probe of molecular organization. Spectral components attributed to DPPC-d62 in cholesterol-rich lo and cholesterol-poor ld phases were observed on the NMR timescale within a certain temperature range. These phases were characterized by determining the order of DPPC-d62, and the relative amount of DPPC-d62 in them. The results demonstrate that this approach is a viable method by which fluid-fluid phase coexistence can be studied. In future experiments, DOPC will be replaced with 1-palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine (PDPC, a PUFA-containing lipid). A similar approach will then be employed to study the effect of PUFA-containing lipids on molecular organization within a physiologically more realistic system.

Poster 18.

Authors: Samuel Canner, Fangqiang Zhu, Scott Feller, Xiaoling Leng and Stephen Wassall

Title: A Role for Lipid-Lipid Interactions in Vitamin E's Function as a Membrane Antioxidant

Vitamin E (α-tocopherol) is the principle lipid soluble antioxidant in cell membranes. Its purpose is to protect membrane lipids from oxidative damage. Whether unequal affinity for different lipids optimizes the proximity of vitamin E to polyunsaturated phospholipids, the lipid species most susceptible to oxidation, is the question that we address computationally with MD simulations on lipid bilayers. Our studies suggest a model that has cholesterol, ubiquitous in the cell membranes of animals, excluding vitamin E from saturated raft-like domains enriched in the sterol. Preferential affinity for polyunsaturated phospholipids is not indicated - vitamin E, like polyunsaturated phospholipids, is pushed towards non-raft regions depleted in cholesterol. The binding energy measured for vitamin E in umbrella sampling AA (all-atom) simulations is less for SDPC (a polyunsaturated lipid) than SOPC (a monounsaturated lipid). Adding cholesterol to SOPC eliminates the differential in binding energy. CG (coarse-grained) simulations run on PDPC (a polyunsaturated lipid) /SM (a saturated lipid)/cholesterol mixtures in the presence of vitamin E indicate the vitamin locates at the boundary between SM-rich/sterol-rich (raft-like) and PDPC-rich/sterol-poor (non-raft) domains. The results of these studies will be presented.

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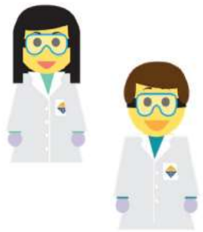

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Poster 19.

Authors: Heidi Kastenholz, Gregory Smith, Anne Wilson and Victor Chen

Title: Case study of green earth pigments as authentic reference materials

In cultural heritage chemistry, it is vital to know what components are present in order to properly care for pieces. In order to properly identify specific materials, a fingerprint match approach to analyses is utilized. In this field, commercial certified reference materials (CRMs) are utilized for comparison. It is documented in previous literature that green earth CRMs contain synthetic pigments, i.e. pthalocyanine green and viridian. Several green earth pigments were evaluated using techniques such as Raman spectroscopy, dark-field microscopy, and X-ray fluorescence spectrometry in order to determine their suitability as CRMs for historic objects.

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Poster 20.

Authors: Armelle Metangmo and Frederique Deiss

Title: Electrochemical paper-based devices for oral preventative care through pH sensing

For the past two decades, many microfluidic paper-based analytical devices have been developed and used in different research fields. These devices are low-cost, portable, flexible, sterilizable, easily disposable, and easy to manufacture. The analytical paper-based devices offer good alternatives to measurements and assays commonly performed in laboratories for analytical and clinical purposes, especially in diagnostics. For example, the determination of pH can be essential in applications in areas as diverse as food industry, agriculture, health care or water treatment. There is a benefit in analyzing the pH in bacterial biofilms formed on teeth (or plaque) as it can be indicative of conditions leading to the formation of cavities. Dental caries is one of the most common chronic diseases world-wide. Cariogenic bacteria thrive in acidic conditions, therefore, assessing the pH of the plaque of a patient can indicate the likelihood of cavities and allow to guide the caregiver for providing preventive care. To address the need for such a pH sensor, we are developing an electrochemical microfluidic paper-based analytical device. We are currently working on an electroanalytical method that involves quantification of pH using stencil-painted graphite electrodes. We have tested solutions with different pH that fall in the cavity-prone range on electrochemical paper-based devices and determined a correlation between the potential of the observed redox peaks and the pH. The next step will involve testing bacterial biofilms cultured on the optimized paper-based devices and assessing interferences that could affect the pH sensing ability of our prototype.

Poster 21.

Authors: Alexander Phillips, Samuel Canner and Stephen Wassall

Title: Unsaturated Lipid Structure and Effects on Membrane Domain Formation

Cell membranes are composed of an enormous variety of lipids and proteins that laterally organize into patches, or domains, of unique composition and function. The lipid raft concept is the most developed model. According to this model, disordered (non-raft) regions composed of primarily unsaturated lipids surround ordered (raft) domains that are enriched in saturated lipids and cholesterol. To study disordered domains, conventional all-atom molecular dynamics (MD)simulations were performed on PLPC (1-palmitoyl-2-linoleoyl-sn-glycero-3-phosphocholine,16:0-18:2PC) and analyzed to study the structure and interactions of this unsaturated lipid that creates a disordered environment. Umbrella sampling was performed on cholesterol in PLPC to determine the binding energy of cholesterol and further evaluate the interactions in a disordered environment. Additional studies were conducted using coarse grained MD simulations on a mixture of membrane lipids comprised of DPPC (1,2-dipalmitoyl-sn-glycero-3-phosphocholine,16:0-16:0PC), DLPC (1,2-dilinoleoyl-sn-glycero-3-phosphocholine, 18:2-18:2PC) and cholesterol. It was observed that the membrane separated into DLPC-rich/cholesterol-poor (non-raft) and a DPPC-rich/cholesterol-rich (raft) domains. The results of these computational studies will be presented.

Poster 22.

Authors: Amara Spencer, Jack Floreancig and Sebastien Laulhe

Title: An Undergraduate Teaching Oriented Approach to Reaction Investigation and Optimization

Peer-Led Team-Learning (PLTL) educational approaches have been shown to increase student’s understanding of content presented to them in a lecture setting. Given the expertise our department has acquired in the incorporation of PLTL to the teaching of organic chemistry, we sought to utilize this method of teaching in the Organic Chemistry II laboratory setting. In particular, we aimed at using a PLTL approach to develop an undergraduate research experience in the model of a CAPSPiE module. Our Peer Lead Undergraduate Research Initiative (PULRI) exposes students to a real research experience led by peer teaching assistants (PTAs). This approach not only benefits the students taking the lab, but also represents a unique research and managerial opportunity for the PTAs. The students conduct all the necessary screens to optimize an organic reaction. Currently students are performing a palladium/copper dual catalysis to form (Pinacolboryl)benzene from bromobenzene. For the past two semesters, we have performed qualitative interviews of the students and PTA’s involved in these new research exposure modules. Both research and educational data will be presented.

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Poster 23.

Author: Ritu Chaturvedi

Title: Hydrazine mediated reverse [2+2] cycloaddition in cyclobutane pyrimidine dimer (CPD)- a synthetic analogue of photolyase catalysed CPD repair

Genomic DNA is under constant attack by a range of exogenous and endogenous agents that cause a covalent modification in its structure. One of the most thoroughly studied DNA lesions is the cyclobutane pyrimidine dimer (CPD). One of the family of pyrimidine photoproducts, CPD is formed by a UV-light promoted [2+2] cycloaddition reaction between two adjacent thymines, resulting in the formation of a permanent cyclobutane ring between the 5, 6-positions. The thymine dimer stalls replicative and transcriptional polymerases, leading to bypass replication by error prone polymerases such as poly η in the former case, and no transcription coupled repair in the latter. In the absence of efficient repair, the thymine dimer lesion can lead to mutation, cancer or cell death.

DNA photolyases are highly efficient blue light-driven DNA repair enzymes, which revert the genome-damaging effects caused by ultraviolet (UV) radiation. CPD photolyases are monomeric proteins of 50-70 kDa that contain two chromophores/cofactors that are non-covalently bound to the apoenzyme. One of these cofactors is always Flavin Adenine Dinucleotide (FAD). The second cofactor is methenyltetrahydrofolate (MTHF) in most organisms and 8-hydroxy-5-deazariboflavin (8-HDF) in a few species that can synthesize this chromophore. The molecular mechanism of DNA repair by CPD photolyase is known in considerable detail, owing to the crystal structures of photolyases from Escherichia Coli and Anacystis nidulans.

Recent findings from our group have led to a chemical reaction that, surprisingly, acts as a synthetic analogue of photolyase-mediated CPD repair. The reaction is mediated by hydrazine and takes places under ambient conditions of temperature and pressure. Current work goes on to explore the kinetics and detailed mechanism of the reaction using UV-Visible spectroscopy, reverse phase HPLC, mass spectrometry and NMR spectroscopy.

Poster 24.

Authors: Jack Floreancig, Amara Spencer and Sebastien Laulhe

Title: Borylation of aryl bromides and iodides using a Pd/Cu dual catalysis

Aryl Boronic esters are important coupling partners in metal-catalyzed cross-coupling reactions as well as a variety of synthetic transformations. Their utility comes from their mild nucleophilicity, high stability, and low toxicity. Traditional methods to synthesize aryl boron reagents require the use of highly reactive reagents such as n-BuLi or stoichiometric amounts of organometallic species such as Grignard reagents. Catalytic methods using transition-metals such as palladium or copper exist, but these methods often lead to competitive homo-coupling byproducts and often require harsh reaction conditions. The major catalytic hurdle within current palladium-catalyzed methodologies is the activation and transmellation step of the diboron reagents, which leads to the use of high reaction temps. To achieve the desired transformations. On the other hand, copper-catalyzed transformations are mainly limited at the oxidative addition step. Therefore, we surmised that using a combination of palladium and copper in a dual-metal catalysis approach would enable facile oxidative addition of palladium to the aryl bromides and iodides, while the copper catalyst would generate a Cu-Bpin species that readily transmetallates. Reaction conditions using aryl bromides and iodides with bis(pinacolato)diboron have been optimized and generate the desired borylated product in good to excellent yields. Substrate scope, functional group compatibility and mechanistic work will be presented.

Poster 25.

Authors: Kiyomi Kukoyi, Carolina Vega and Frederique Deiss

Title: Electrochemical Detection of Chlorate Using Paper-based Devices for Crime Scene Investigation

In recent years, more and more improvised explosive devices are made with chlorate salts. This is due to chlorate salts being easier to use and buy, submitted to less regulations than other common oxidizing agents such as ammonium nitrate. For forensic applications, in-field presumptive sensing capabilities are needed. Microfluidic paper-based analytical devices are low-cost, portable, flexible, and simple to produce and to use, and can be used for sample collection. We are developing an electrochemical paper-based device to detect and quantify the presence of chlorate using a molybdate sensing layer. The redox reactions of the molybdate are catalyzed by chlorate and, thus, shifts in the peak of potential and increases in current can be observed by electro-analytical techniques such as cyclic voltammetry. Our current work is focused on exploring the best conditions for the electrodeposition of the molybdate layer and the detection of chlorate, such as the scan rate and device design. We are also exploring various methods of data analysis to more conclusively display the impact of chlorate on the sensing layer. Current experiments are focused on determining the most effective and efficient way to electrodeposit the molybdate sensing layer. Completing optimization of these devices will allow us to begin testing with real samples (pipe bomb debris) collected in May 2018. This project aims to permit a convenient collection and analysis of samples (explosives mixture or debris) for investigators at crime scenes.

Poster 26.

Authors: Bryant Kim and Jingzhi Pu

Title: Assessing Force Matching QM/MM Models for Computing Solution Phase Free Energy Profiles

Force-matching models in chemical reactions offer an alternative strategy for updating approximated semiempirical methods to converged accurate free energy surfaces at high accuracy ab initio (AI) levels. With this strategy we compare a force fitting model which constructs the pairwise potential based on an approximated power series with the previously developed reaction path force matching in collective variables (RP-FM-CV) model. In essence, forces which are linearly combined from a constructed pairwise potential are compared with forces fit to a spline interpolation function. For the two-dimensional reaction coordinate of the Menshutkin and Finkelstein reactions, the quality of force matching is assessed by decomposing the free energy contributions of each CV along the reaction coordinate. In this study we demonstrate force matching as reaction coordinate specific instead of having a well-defined function. With the recent developments in force matching strategies, we plan to investigate multi-dimensional biological reaction coordinates to better understand the mechanisms and functions of complex solution phase reactions.

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Poster 27.

Authors: Shivansh Mahajan, Rachel Cadle, Julie Dinh, Chloe Gonterman, Verena Haug, Bruce D. Ray and Michael J. McLeish

Title: Evaluating the individual roles of active-site residues of benzoylformate decarboxylase

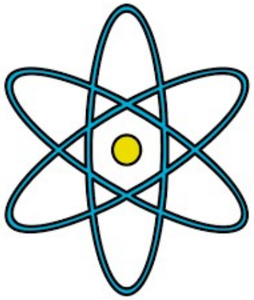
Benzoylformate decarboxylase (BFDC) is a thiamin diphosphate (ThDP)-dependent enzyme, initially isolated from Pseudomonas putida, which catalyzes the decarboxylation of benzoylformic acid yielding benzaldehyde and carbon dioxide. As a side reaction, BFDC also exhibits carboligase activity, catalyzing the formation of stereospecific α-hydroxy ketones that are of interest as precursors to pharmaceuticals. Based on mutagenesis studies, three active site residues, Ser26, His70 and His281 are known to play important roles in the catalytic mechanism of BFDC, but their precise roles are still in dispute. Some clarity was provided by a recent modeling study (Planas et al., Front. Chem 6, 2018; doi:10.3389/fchem.2018.00205), but more definitive evidence is still required. In this project, we have analyzed the contributions of the three residues to individual catalytic steps. Select active site variants were over-expressed in E. coli and purified using Ni2+ affinity chromatography. Initially, the steady-state parameters of the variants were determined using a NADH-linked coupled assay. Then, a combination of rapid chemical quench and 1H NMR spectroscopy was used to determine the relative concentrations of reaction intermediates at steady state and, ultimately, rate constants for those intermediate steps. Here, we report those results and discuss their implications.

Poster 28.

Authors: Andrew Riley, Seyyedamirhossein Hosseini and Zhihai Li

Title: Photoelectrochemical properties and photocatalytic effect of doping nickel tungstate with group 11 elements

Nickel tungstate (NiWO4) has been well studied for its role as a photoactive semiconductor. Its large surface area makes it an idea candidate for catalytic use, and it has even been investigated for its ability to convert sunlight into usable energy. Nickel Tungstate has shown the capacity to effectively convert sunlight (solar energy) to electricity. Our research involves doping of nickel tungstate with 3%, 6%, and 9% copper or silver in order to investigate its effect on nickel tungstate as a photovoltaic (PV) material, as well as a photocatalyst for degradation of organic contaminants in wastewater. Doped NiWO4 was be prepared and characterized with different techniques such as atomic force microscopy (AFM), transmission electron microscopy (TEM), x-ray photoemission spectroscopy (XPS), and x-ray diffraction (XRD). Future studies will investigate the photoactivity of these doped compounds, both for photocatalytic and photovoltaic applications.



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Poster 29.

Authors: Nicholas Ensinger and Elsayed Zahran

Title: Light-Activated Degradation of Glyphosate by Palladium-Decorated m-BiVO4/BiOBr Nanosheets

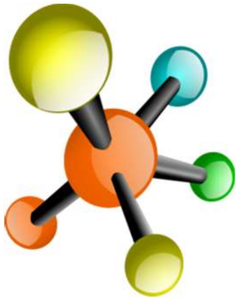
Glyphosate (N-(phosphonomethyl)glycine) is one of the most widely used herbicides in the United States and was found to be persistent in the environment. Recently, glyphosate was classified as a potential carcinogen and was related to the disruption of gut bacteria in honey bees. In this poster, we report the light-activated catalytic degradation of glyphosate by Pd/m-BiVO4/BiOBr photocatalyst. We prepared the ternary composite photocatalyst Pd/m-BiVO4/BiOBr according to our previously reported one-pot synthesis. The photocatalytic activities of the bare m-BiVO4/BiOBr and the Pd-decorated particles, with various Pd content, were elucidated via the degradation of rhodamine B. These materials were employed in the photocatalytic degradation of glyphosate and subsequently aminomethylphosphonic acid (AMPA), under simulated sunlight irradiation. The kinetics of the photocatalytic degradation reaction was studied by monitoring the concentration of glyphosate and its degradation products by ion chromatography. Complete degradation of glyphosate by Pd/m-BiVO4/BiOBr was achieved within 5 minutes of the reaction. Such results could lead to the development of sustainable catalytic technologies to minimize the global impact of glyphosate.

Poster 30.

Authors: Charles Irving, Makafui Gasonoo and Sebastien Laulhe

Title: Direct Acyl Amide Synthesis from Carboxylic Acids Using N-Haloimide Reagents

Acyl phthalimides and amides are important classesd of compounds since they are precursors to biologically active compounds, natural products and even polymers. Current methods of acyl phthalimide and amide synthesis range from the use of pre-generated phosphonophthalimide reagents with carboxylic acids, acyl substitution reactions of carboxylic acids and their derivatives, and metal catalyzed cross coupling reactions. While effective, such methods require the synthesis of commercially unavailable reagents, toxic/water sensitive substrates, and expensive metal catalysts, respectively. Therefore, the design of metal-free reactions using stable and commercially available carboxylic acids would represent an attractive approach to the synthesis of acyl phthalimides and amides. We hypothesized that the in situ synthesis of chlorophosphonium salts from N-chloroimides and triphenylphosphine could serve as an effective amination and coupling agent for the formation of acyl phthalimides and amides. Aliphatic, aromatic, benzylic, and allylic carboxylic acids were all observed to be suitable substrates for acyl phthalimide and amide synthesis. Aliphatic, aryl, and benzylic primary/secondary amines were found to serve as suitable substrates for amide synthesis as well. Substrate scope, robustness of the reaction, as well as functional group compatibility and mechanistic work will be presented.



Poster 31.

Authors: Kyle Colston, Sara Dille and Partha Basu

Title: Probing the Charge Transfer Properties of Asymmetric Molybdenum Dithiolene Complexes with DFT

Excited state transitions of asymmetry molbydenum(IV)-oxo complexes with thiophenol (SPh), 1,2 benzenedithiol (bdt), and N,N'-dimethyl piperazine 2,3 dithione (Me2Dt0) ligands have been modeled using time-depended density functional theory (TD-DFT). Calculations were performed using B3LYP/6-31G(d,p)/LANL2DZ level of theory in both gas phase and solvated models (PCM). Geometries were obtained via gas phase geometry optimizations and atomic orbital contributions determined via C-squared population analysis. Low energy charge transfer bands were determined to be predominantly ligand-to-ligand charge transfers (LL'CT) in which the electron rich dithiolene ligand acts as donor and the electron deficient dithione ligand participates as the acceptor.

Poster 32.

Authors: Alexandria Mossbarger, Zachary Krawczyk, Charles Irving and Sebastien Laulhe

Title: One-Pot Oxidation of Amines From Phosphine-Activated Benzoyl Peroxide

Amides are an important class of compounds and acts as precursors for pharmaceutical drugs, insecticides, and polymers. Common methods for amide synthesis involve reacting amines with carboxylic acids in presence of activating agents, or via acyl substitution. While such methods are robust and efficient, they sometimes require multiple reaction steps and the use of toxic reagents. The design of a metal-free methodology using cheap, stable, and commercially available starting materials in one-pot, would represent an attractive alternative to amide synthesis. We hypothesized that benzoyl peroxide when reacted with a phosphine activator, would generate a phosphonium intermediate that would allow for amide formation when introducing an amine nucleophile. Such a reaction would not require the use of a base. The method was shown to be efficient for a variety of primary and secondary amines including; aliphatic, aryl, benzylic, bifunctional, and cyclic substrates. Substrate scope, robustness of the reaction, as well as functional group compatibility and mechanistic work will be presented.

Poster 33.

Authors: Fizzah Qureshi and Tien-Min G. Chu

Title: The design, chemistry, fabrication, and application of a load-bearing tissue engineering scaffold

Biodegradable scaffold plays several critical roles in tissue engineering, including a temporary structure for cell attachment, as a reservoir for growth factors and, and as a carrier for cells. Typical scaffold are highly porous to allow for nutrient diffusion and space for cell proliferation. However, in long bone tissue engineering, a scaffold capable of bearing load is critical to allow participation in the initial load bearing function along with the fixation hardware. For these reasons, we have developed a load bearing tissue engineering scaffold from poly(propylene) fumarte/tricalcium phosphate (PPF/TCP) biodegradable composite in a general shape of a solid cylinder. Since long bone heals by forming a callous around the defective area, a porous structure was not needed. The design allowed the scaffold be used in conjunction with two common long bone fixation techniques: either bone plate fixation or intramedullary pin fixation. Release of multiple drugs from the scaffold was also possible through the use of dicalcium phosphate dihydrate cement in the side portal of the scaffolds. In this poster, the chemical components of the scaffold materials, the geometry and engineering design of the scaffold, fabrication method, potential degradation process, and applications of scaffolds in various studies are presented.

Poster 34.

Authors: Maria Barron, Monica Barron, Tiyash Bose, Daniel Debroye, Michael Pugia and Frederique Deiss

Title: Electrochemical Detection of Bacteria by Alkaline Phosphatase labeled Antibodies

Bacteria are a very common and sometimes life-threatening source of illness around the world. In 2016, respiratory infections and diarrheal diseases were among the top ten global causes of death. One of the most common types of bacterial infections is urinary tract infection (UTI.) Early determination of the presence and type of bacteria present can allow for better treatment of infectious diseases. In particular, differentiation between gram positive and gram negative bacteria dictates the appropriate treatment method, as these two types of bacteria are susceptible to different antibiotics.

The goal of this project is to detect the presence and type of bacteria in urine using an electrochemical device within a microfluidic system. The bacteria will be screened for by the selective binding of antibodies labeled with enzymes that produce electrochemically active products. The chosen enzyme for the detection of the presence of bacteria is alkaline phosphatase, which converts p-aminophenol phosphate (PAPP) to p-aminophenol (PAP) in alkaline conditions. Our group seeks to design a detection method by the optimization of the enzyme and substrate concentrations, the comparison of different electrochemical platforms, and the selection of the optimal pH for the multiplexing of alkaline phosphatase with other enzymes.

Poster 35.

Author: Ryan Young

Title: Implementation of Polarizable Intermolecular Potential Functions in CHARMM

Intermolecular electrostatic polarization plays an important role in understanding many condensed-phase physical and chemical phenomena. Conventional force fields used in computer simulations, however, lack explicit description of intermolecular polarization, which makes the development of polarizable models a central theme in designing the next-generation force fields. Here we present an implementation of polarizable intermolecular potential functions (PIPFs) employing the interacting point-dipole approach. The PIPF approach enables intermolecular polarization by introducing a set of atomic polarizabilities, based on which the induced dipoles on atomic centers are determined self-consistently. In our implementation, the interacting centers participating in the induced-dipole calculations are conveniently obtained by making use of the non-bonded interaction pair list constructed in the CHARMM program for conventional molecular dynamics simulations. To validate our implementation, we conducted constant-temperature constant-pressure molecular dynamics liquid simulations based on the POL2 polarizable water model as well as the TIP3P non-polarizable water model. Comparison of the polarizable and non-polarizable simulations on various water properties including dimer geometry/binding energy, density, heat of vaporization, self-diffusion constant, and radial distribution function, suggests improvement of the polarizable model in reproducing experimental results.

Poster 36.

Authors: Kent Shilts and Christoph Naumann

Title: Examining cell migration and cell junction dynamics using a polymer gel-tethered lipid bilayer

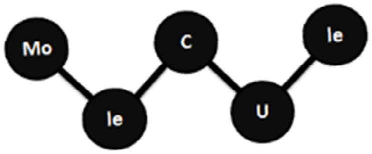
Fate and function of anchorage-dependent cells depend on multiple environmental cues, including those of mechanical origin. Cells probe external mechanical cues through cellular adhesions, such as focal adhesions and adherens junctions, which act as responsive mechanosensors. Previous progress in the understanding of cellular mechanosensitivity can be attributed to the availability of linker-functionalized polymeric gels of adjustable stiffness, which mimic extracellular matrix (ECM) conditions. However, such ECM mimetics are limited in their ability to replicate the remarkable plasticity and dynamics found at cell-cell junctions. To overcome this shortcoming, here we introduce the cadherin functionalized polymer gel-tethered lipid bilayer (PGTB) as an improved cell-to-cell contact mimetic. Its key features include: (i) the dynamic assembly of linker molecules into clusters at cell-induced adhesion sites, enabling cell spreading and migration, and (ii) the ability to alter substrate stiffness by changing the composition of the underlying polymer gel. Data from fluorescence correlation spectroscopy (FCS) and spot photobleaching experiments show the lipid bilayer has lateral mobility, which is a hallmark of the plasma membrane. Experimental findings show that adherent cells on PGTB substrates of varying gel stiffness exhibit markedly different global properties of cellular mechanosensitivity (i.e., cell area, migration speed, and cytoskeleton organization). Furthermore, cadherin clusters underneath plated cells show long-range lateral mobility with remarkable similarity to the dynamics of cell-cell junctions in cell clusters. These results illustrate that PGTBs are an advanced mimetic of the cell surface and allow cellular mechanosensitivity in cell-to-cell junctions to be investigated.

Poster 37.

Authors: Ben Dawson and Dr. Annie Wilson

Title: Strategies toward the synthesis of Juliet Blue

Triarylmethane dyes are a historically important and chemically interesting class of compounds in the area of dye and pigment chemistry. In the synthesis of our triarylmethane target, Juliet Blue, we utilized various redox reagents in the presence of precursor quinolone compounds to investigate the mechanism of the formation of this target, as well as optimize the amount of target isolated. In addition to the synthetic approaches, the complete spectroscopic characterization of our target compound will be discussed.



Poster 38.

Authors: Ashur Rael, Magnus Rydberg, Courtney Cruse and John Goodpaster

Title: Gas Chromatography/Vacuum Ultraviolet Spectroscopy (GC/VUV) versus Gas Chromatography/Electron Ionization Mass Spectrometry (GC/EI MS) for C1, C2, and C3 Alkylbenzenes

Gas chromatography (GC) coupled to Mass Spectrometry (MS) is the standard method for forensic analyses of ignitable liquid residues and many other types of analysis. Recently, a new type of GC detector, a vacuum ultraviolet (VUV) spectrometer, has become commercially available in the 120-430 nm wavelength range, spanning the far UV to the blue visible wavelengths. Originally developed to meet the needs of the petrochemical industry, this detector is currently being evaluated for its broader utility in analytical chemistry due to the higher energy molecular transitions it can detect. The addition of the 120-160 nm range allows detection σ to σ* transitions, like those for alkyl groups. The specificity exhibited by these VUV detectors is due to their ability to probe energy transitions that are characteristic of structure: σ to σ*, n to σ*, π to π*, and n to π*. VUV detection has the potential to readily differentiate molecules that yield similar or identical mass spectra. While the mass of structural isomers does not change between isomers, the differences in molecular energy transitions can be measured. VUV detection is also nondestructive and does not suffer from the low abundance of the molecular ion which can trouble EI MS analysis of some molecules. Previous work has shown that the combination of VUV and MS detectors results in improved library matches for volatile organic compounds. Here, we utilize a GC with VUV and a GC with an EI MS detector and evaluate their individual performance for differentiating and identifying aromatic structural isomers (e.g., o-,m-,p-xylene) found in common ignitable liquids and their residues. Furthermore, we compare the qualities of two detection methods for quantitation.

Poster 39.

Authors: Carolina Guimaraes Vega, Kiyomi Kuyoki, David Wilkins, Daniel Collins and Frederique Deiss

Title: Electrochemical Paper-based Sensor for the Trace Detection of Chlorate in Crime Scenes

Improvised explosive devices (IEDs) are deadly weapons that are particularly dangerous as they can be done from unsuspected components, such as every-day life objects and household chemicals. An increasing number of IEDS using chlorate salts as oxidizer have recently been reported. The tools to detect chlorate in the field are however limited. To address the current need for on-site chlorate detection, we are developing an electrochemical paper-based device to detect and quantify chlorate. Microfluidic paper-based devices are low-cost, portable, disposable, and simple to produce and use. Chlorate was reported to have a catalytic effect on the redox reactions of molybdate. Our sensing platform will detect chlorate by monitoring the change in redox activity of the molybdate sensing layer using electro-analytical techniques such as cyclic voltammetry. We are currently optimizing the conditions (pH, type of acid, scan rate, concentration of molybdate, etc.) for the electrodeposition of molybdate sensing layer and the detection of chlorate. We have successfully demonstrated the detection of chlorate in solution and started assessing the quantification capabilities of the device. These devices will allow a convenient sample collection at crime scenes, in-field presumptive test, storage and transport to laboratory for further confirmatory tests.

Poster 40.

Authors: Alex Griebling and Roderick Macrae

Title: Effect of the Interaction of Metal Salt Cations on Glucose α/β Anomer Ratios

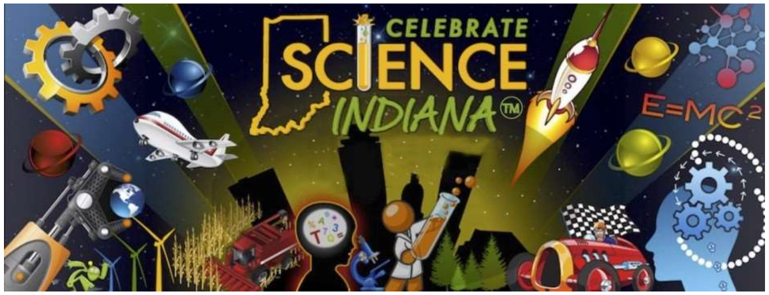
Simple sugar behavior in solution has been studied over the past 150 years to understand the effects of various parameters, including temperature and solution concentration, on anomer formation in equilibrium conditions. One area that lacks elucidation is the effect of metal salt cations on anomeric ratios of glucose. D-Glucose, the biologically active form of glucose, exhibits a simple monosaccharide structure that, when undergoing mutarotation, reacts slowly into two anomer forms: α-D-glucose and β-D-glucose. α-D-glucose and β-D-glucose differ from the position of a hydroxyl group. 1M D-glucose solutions were reacted with different concentrations of metal cationic solutions to determine the ratio between α-D-glucose and β-D-glucose: lithium chloride (LiCl), sodium chloride (NaCl), magnesium chloride hexahydrate (MgCl*7H2O), and calcium chloride (CaCl2). Polarimetric data suggests that LiCl and NaCl do not change the phase angle, while MgCl*7H2O and CaCl2 cause more notable changes to the phase angle. This indicates that the larger cation may induce more of an influence on the ratio of α-D-glucose and β-D-glucose. Nuclear magnetic resonance (NMR) data is being studied for small changes in spectra to determine the effect of metal cationic salts on the α/β anomer ratio.

Poster 41.

Authors: Sean Dunlap and Phillip Albiniak

Title: An Exploration of the Solubility and Recovery of Oxypyridinium Salt Byproducts

Benzyl ethers are useful protecting groups for alcohols due to their durability under a variety of reaction conditions and facile removal under mild conditions. The primary drawback to the usage of benzyl ethers has been the harsh conditions required for their synthesis. 2-benzyloxypyridinium triflate or Dudley salt was created to overcome this limitation. Specifically, the Dudley salt reacts in an SN1-like mechanism in which the salt decomposes to generate a benzyl cation under the application of heat allowing for nucleophilic capture with an alcohol. Based on this mechanism, several derivatives have been produced from the original Dudley salt by either changing the transfer group or modifying the overall functionality of the salt. Due to the additional steps needed to synthesize these derivatives, they are significantly more expensive than the original reagent. The work presented here focuses on the exploration of the recovery and isolation of the salt byproduct after a reaction by manipulating the byproduct's solubility. With the byproduct in hand, reforming the salt from the byproduct to make recyclable oxypyridinium salts will be investigated to make these reagents more cost effective and efficient.

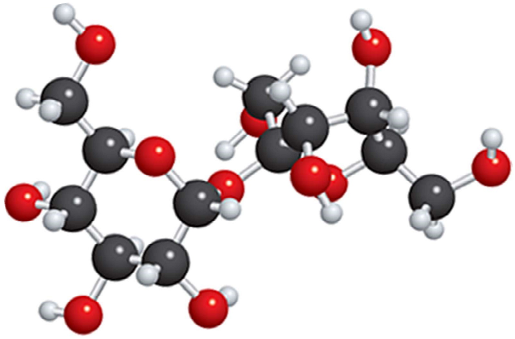


Poster 42.

Authors: Charles Sexton and Nicholas Manicke

Title: Shotgun Proteomics by Paper Spray Mass Spectrometry

Shotgun proteomics refers to the method used to identify proteins by their fragment peptides collected via proteolytic digestion. As with top-down proteomics, post translational modifications and mutant variants can be identified. Hemoglobin mutations such as HbC, HbD, HbE, and HbS can be detected from the tryptic peptides of intact hemoglobin found in whole blood samples. Engineered toxoids akin to recombinant staphylococcus enterotoxin B (SEBv) can have their amino acid substitutions, such as L65R, confirmed by studying the resulting peptides of an enzymatic digestion. Parvalbumin proteins found in fish can be used to differentiate closely related species. In each of the cases above, shotgun proteomics by PS-MS/MS was performed on a Q-Exactive Orbitrap allowing for a rapid analysis of peptides with high mass accuracy and precision. Unique peptide fragments obtained from enzymatically digested proteins using immobilized trypsin on a nylon membrane was used to confirm the presence or absence of mutations in hemoglobin, modifications in SEBv, and specific parvalbumin proteins in fish species.



Poster 43.

Authors: Chris LeMasters

Title: Kinetic studies of oxypyridinium salt transfer reactions towards new reagent development

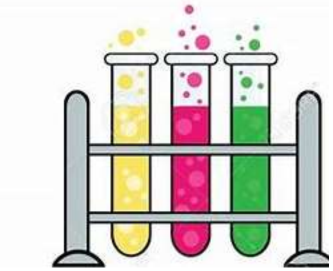
New reagent synthesis and design is an important route to developing new synthetic methods. For example, 2-benzyloxy-1-methylpyridinium triflate (BnOPT) was first reported as a benzyl transfer reagent in 2006. Since then, it has found a niche as a powerful benzyl electrophile that can be quenched with various nucleophiles under mild conditions without the need for acidic or basic additives. More recently, a variety of derivatives have been synthesized which can transfer alternative functionality including halobenzyls, p-methoxybenzyl, allyl, and t-butyl groups. However, in order to make these oxypyridinium salts as broadly useful as possible, a more complete understanding of the mechanism of transfer is required. Preliminary evidence of these substitution reactions indicate a more SN1-like mechanism in which the salt decomposes to a cation first, followed by nucleophilic trapping in a second step. The focus of this study includes an examination of the kinetics of the transfer reaction with a variety of substituted aryl oxypyridinium salt derivatives. This poster will show the development of a reliable technique for monitoring these transfer reactions by 1H NMR. This data will ultimately be used in a Hammett plot to give a clear indication of how much cation character is being developed at the benzylic carbons of these salts.

Poster 44.

Authors: Veeda Scammahorn, Yuna Lee and Kelsey Scott

Title: One-Pot Synthesis of Disubstituted Malononitrile Derivatives

Forming carbon-carbon bonds selectively can be a challenging task in synthetic organic chemistry. Previously, our laboratory has determined that the Knoevenagel condensation of malononitrile with a range of aromatic aldehydes can be done efficiently in ethanol and sodium borohydride is a good reagent for reducing the product to deliver monosubstituted malononitriles in a single reaction flask. This research develops a new synthetic one-pot procedure for the synthesis of disubstituted malononitrile derivatives creating two new carbon-carbon bonds. The final malononitrile derivatives can be utilized as the basic unit for pharmaceutical and agricultural chemicals or as synthetic intermediates to useful heterocycles.



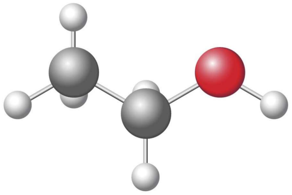
ACS Local Section
Indiana

Poster 45.

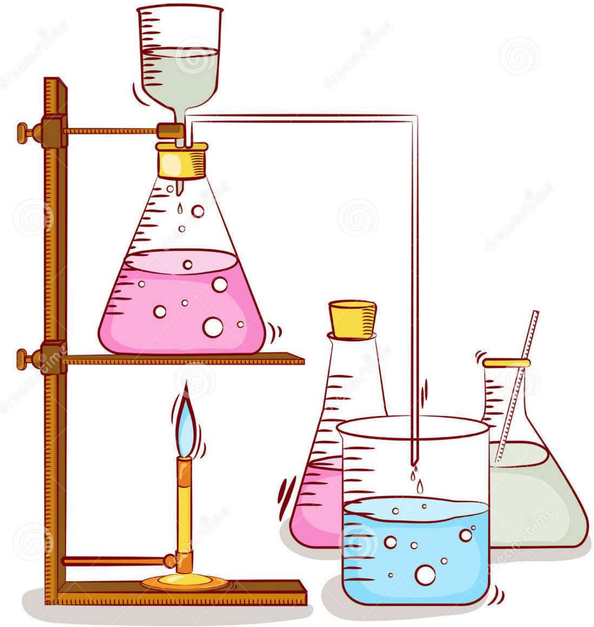
Authors: Wei Wei, Colin J. Wallace, George C. McBane, Carolyn E. Gunthardt, and Simon W. North

Title: Photodissociation Dynamics and Vector Correlations of OCS

The photodissociation dynamics of carbonyl sulfide (OCS) near 214 nm has been studied to help improve models for the gas phase photochemistry. The goal is to explore the effects of shorter wavelength on photodissociation dynamics and how much impact does it have on our understanding of photochemistry. OCS photodissociation at the first absorption band has been studied for more than 20 years with both experimental and computational methods. Previous studies show that the dominant dissociation channel produces 1D state sulfur and ground electronic and vibrational state CO molecules with high rotational excitation. A mechanism has been proposed to explain the product distributions. But no studies have been reported on the short end of the absorption band. A velocity map ion imaging apparatus in Texas A&M University has been employed to make comprehensive measurements of both photo-product distribution and signatures of excited state involved at photodissociation near 214 nm. The photo-product rotational distributions near 214 nm show generally similar trend compared to those at longer wavelength, while a significant ratio of vibrationally excited CO product channel is observed.1 These results reveal a new challenge for future theoretical chemistry research.



Thank you for attending the Think Like A Molecule Poster Session!!



Please remember to fill out an evaluation to be entered in the raffle for some great prizes!

2020 Think Like a Molecule Poster Session
part of the
IU Bicentennial Anniversary

Collaborating Associations/ Organizations/ Academies conference

Beyond Boundaries: Indiana Academies Symposium 2020

(Fri-Sat.) April 3-4, 2020; Indiana Convention Center

ACS coordinated events are shown below.

Day One (Friday, April 3, 2020)

10:30 am – 12:00 am	Symposium special collaborations – oral
12:15 pm – 1:30 pm	Networking lunch
1:45 pm – 3:15pm	Oral presentations from students 1
3:45 pm – 4:45 pm	Oral presentations from students 2
4:45 pm – 5:00 pm	Reception/Poster Sessions
6:45 pm – 8:30 pm	Major Keynote address and Conference Banquet
8:30 pm – 10:00 pm	Ice cream social/networking night

Day Two (Saturday, April 4, 2020)

10:30 am – 3:15 pm **Think Like a Molecule 2020** (annual poster session) with 2 poster sessions, a lunch with keynote speaker and awards ceremony

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October 5, 2019

ACS Illustrated Poem Contest
2019 Theme

Save the Date

Marvelous Metals

NCW 2019 explores the properties and uses of metals

http://www.acsindiana.org/acs/

Electronic Submissions due by **9-19-19**

4 categories: K-2, Grades 3-5,Grades 6-8, Grades 9-12

Prizes: 1st Place = \$100, 2nd Place = \$50, and 3rd Place = \$25 in each age group.

Online Resources

American Chemical Society: http://www.acs.org
IUPUI school of science: http://science.iupui.edu
NOBCChE: https://www.nobcche.org/
Group on Graduate, Research, Education, and Training (GREAT): https://www.aamc.org/members/great/
Medical Minority Applicant Registry (Med-MAR): https://www.aamc.org/students/minorities/med-mar/
Professional Networking: https://www.linkedin.com/
Strengths Finder: http://www.strengthsfinder.com/
Job Opportunities and Resources:
    http://www.idealist.org/
    http://www.indeed.com/
    http://www.glassdoor.com/
    www.forbes.com/sites/.../09/.../the-top-75-websites-for-your-careeer

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High School Summer Research Program

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Project SEED was established by the American Chemical Society in 1968 to give high school students the opportunity to explore a career in the sciences and be involved in research at industries and universities. The Indianapolis program began in 1973 at the IU School of Medicine.

http://www.indyprojectstem.org/

Contact Program Director Elmer Sanders at (317) 514-3212 or elmer.sanders@yahoo.com

2018 Winners

ACS-IUPUI Poster Session Award Winners

Grand Prize Winner - Ritu Chaturvedi, IUPUI

ACS Project Seed Poster Presentation Award

- First Place: Sherlyn Contreras- Project SEED HS Student

ACS Chair's Poster Presentation Award

- First Place: Mark Woollam- IUPUI
- Second Place: Clayton Westerman- Ball State
- Third Place: Alexander Latta- IUPUI
- Honorable Mention: Armelle Metangmo- IUPUI
- Honorable Mention: Ashur Rael - IUPUI

IUPUI Dean's Poster Presentation Award

- First Place: Bryant Kim- IUPUI
- Second Place: Charles Irving- IUPUI
- Third Place: Slade Kepler- Ball State
- Honorable Mention: Tori Goldsworthy– Ball State
- Honorable Mention: Tyler Williams– Ball State

Kurek Student Poster Presentation Award

- First Place: Zachary Thom- IUPUI
- Second Place: Alexandra Kelley- IUPUI
- Third Place: Magdelana Stinnett- IUPUI
- Honorable Mention: Macon Shroyer – Ball State

http://www.acsindiana.org/acs/2018/04/19/think-like-a-molecule-poster-session-awardees/