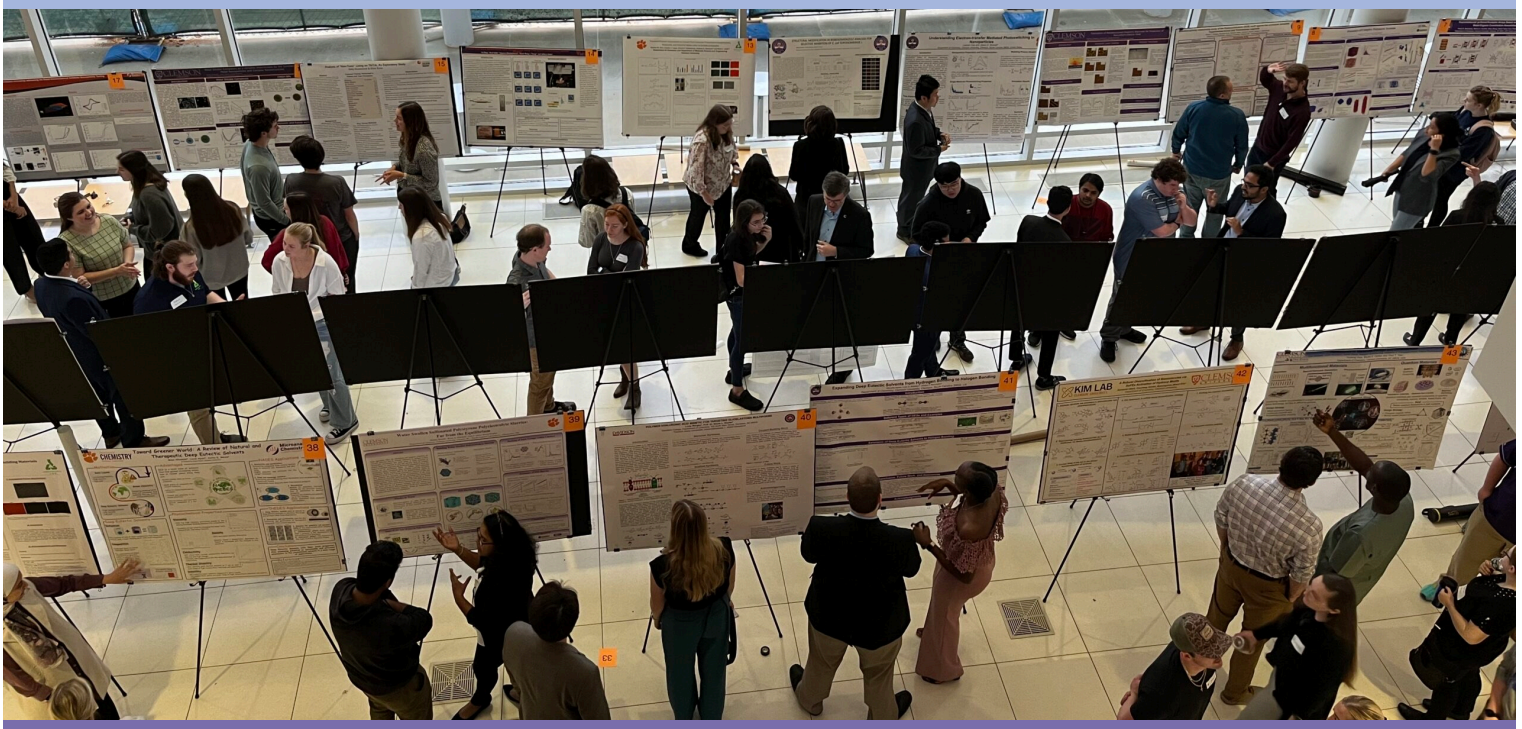
Clemson Chemistry Department
9th Annual Research Symposium

Saturday Feb 24, 2024
9:00 am - 12:00 noon
Watt Family Innovation Center, Clemson University



Keynote Address: Immunoassays and Disease Diagnostics: It's Not Just About Limits of Detection

Prof. Marc D. Porter
Chemical Engineering and Chemistry
University of Utah

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We would like to specially acknowledge the financial support provide by the following organizations:

Message from the Chair

Dear Faculty, Staff, Students and Honored Guests,

Welcome to the 9th Chemistry Research Symposium, which highlights research performed at Clemson by our students and at other institutions by our honored guests. All of these students have worked very hard to highlight the variety and importance of research being done in chemistry. Interact with the poster authors and experience the enthusiasm and dedication they have for their work. Enthusiasm is contagious, and we hope that you will be inspired by your conversations with them to want to know more. Science isn't hard work for the curious, but it does provide education and training for a wide variety of careers and vocations, and chemistry, as the central science, provides a jumping off point to a world full of opportunities.

We hope you enjoy your time with us!

Bill Pennington

Keynote Speaker

Dr. Marc Porter
University of Utah

Immunoassays and Disease Diagnostics: It's Not Just About Limits of Detection

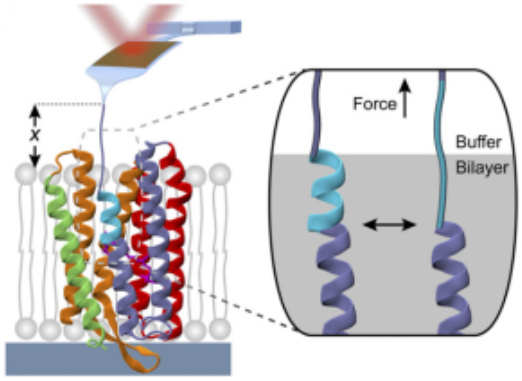
The drive for early disease detection, the growing threat of bioterrorism, and the need for safe and secure food and water supplies have amplified the demand for ultrasensitive, high-speed diagnostic tests.
This presentation will describe our efforts to develop platforms and readout methodologies that potentially address these needs by coupling nanometric-labeling concepts based on surface-enhanced Raman scattering (SERS) and giant magnetoresistance (GMR) readout. It will focus on the impact of what are often called preanalytics, or the handling and preparation of patient and other types of specimens, on the clinical utility of the measurement. Findings that point to the importance of sample pretreatment with respect to the exacting measurement of biomarkers for tuberculosis diagnostics, and pathogens like *Salmonella* spp, anthrax, and *E. Coli* O157-H7 will be examined. Possible implications of these results will also be discussed.

Book of Abstracts

Poster #1

Single-Molecule Studies of Membrane Proteins

Abideen Ayangbemi (a), Christopher Hatchell (a), and David R. Jacobson (a)
(a) Department of Chemistry, Clemson University

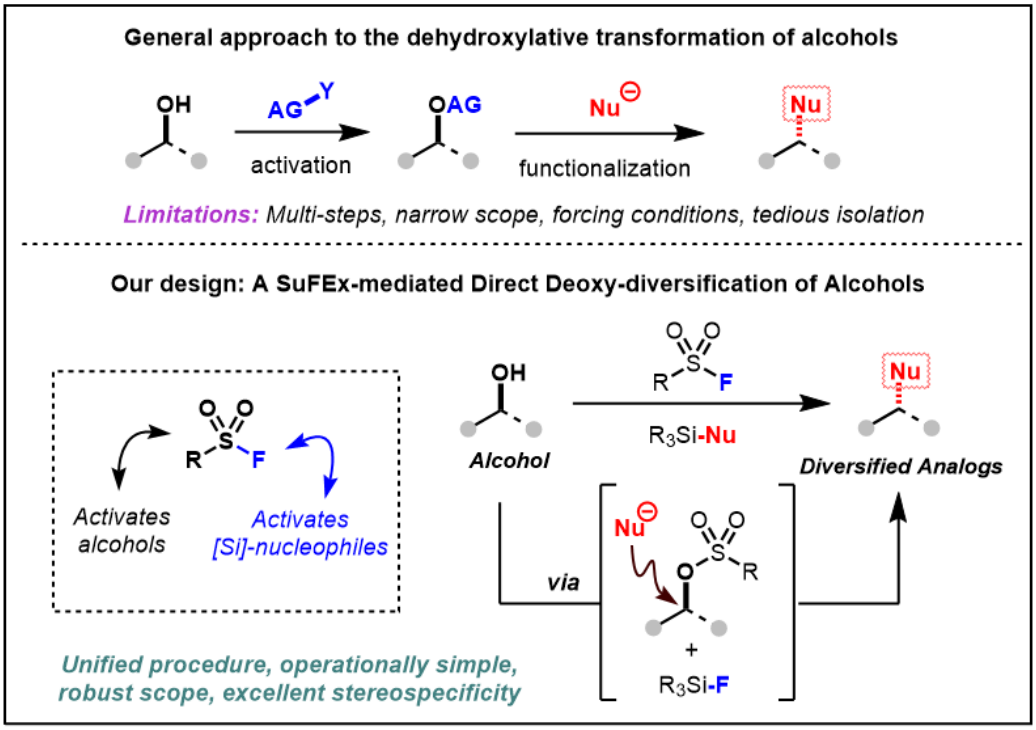


Membrane proteins (MP) are present on the surface of cells, which make them important targets for therapeutics that alter signaling pathways. Investigation of the structure and energetics of membrane proteins has yielded breakthroughs in recent years but still faces several challenges. A promising new approach to thermodynamic characterization of MPs involves single-molecule measurement of near-equilibrium unfolding and refolding induced by mechanical force applied using an atomic force microscope (AFM). We are developing novel methods to obtain biologically relevant information from such single-molecule studies. We are modifying commercially available cantilevers using focused-ion-beam lithography to achieve sufficiently fast time response to measure these folding transitions. We are developing methods to mimic or reproduce the native lipid bilayer in such studies, including detergent-free solubilization, naturally occurring outer membrane vesicles, and polymer nanodiscs. We are applying these methods to disease-linked human proteins that cannot be studied using conventional biochemical methods.

Poster #2

Deoxy-Diversification of Alcohols via SuFEx-mediated Activation of Substrates and Nucleophiles

Amaechi Odoh, and Dr. Byoungmoo Kim
Department of Chemistry, Clemson University

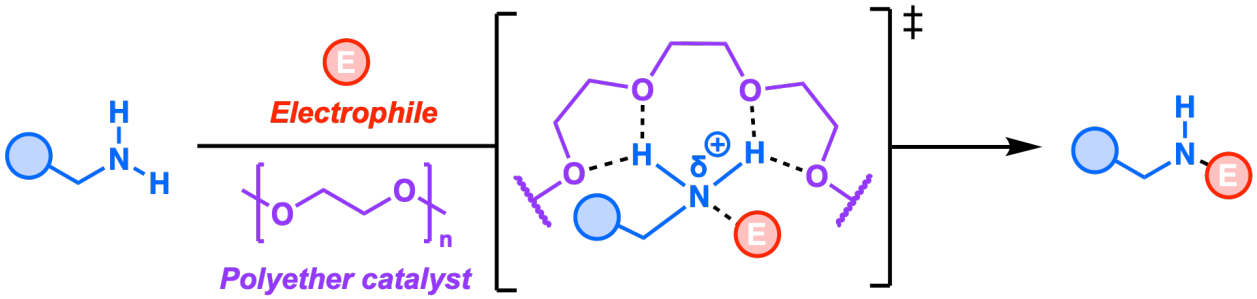


Hydroxy groups, which are prevalent in natural products and biomolecules, stand as prime targets for biomolecular diversification because they facilitate the adoption of deoxy-functionalization as a versatile synthetic avenue for constructing compound libraries possessing unprecedented biological properties. However, existing deoxy-functionalization methodologies encounter several drawbacks, such as competing elimination reactions, lack of stereospecificity, limited efficiencies, and a narrow scope. As part of our ongoing study on the development of practical and efficient deoxy-functionalization of alcohols, we demonstrate herein a unified deoxy-diversification protocol in which a single reagent activates alcohol substrates and nucleophiles via Sulfur(VI) Fluoride Exchange (SuFEx). This pioneering technique facilitates the conversion of alcoholic C,ÄìO bonds in natural products and biomolecules into an extensive array of diversified analogs featuring other bond types such as C,ÄìC, C,ÄìN, C,ÄìCl, and C,ÄìBr. Additionally, the transformation proceeds under mild conditions, thereby ensuring wide-ranging substrate compatibility and a high functional group tolerance. Hence, it holds great promise for accelerating drug discovery campaigns and for delving into the uncharted territory of nature's molecular diversity.

Poster #3

Catalyzed Enhanced Reactivity of Amines Through Weak Noncovalent Interactions

Andrew Storer (1), Amaechi Odoh (1), Austin Seilkop (1), and Byoungmoo Kim
(1) Department of Chemistry



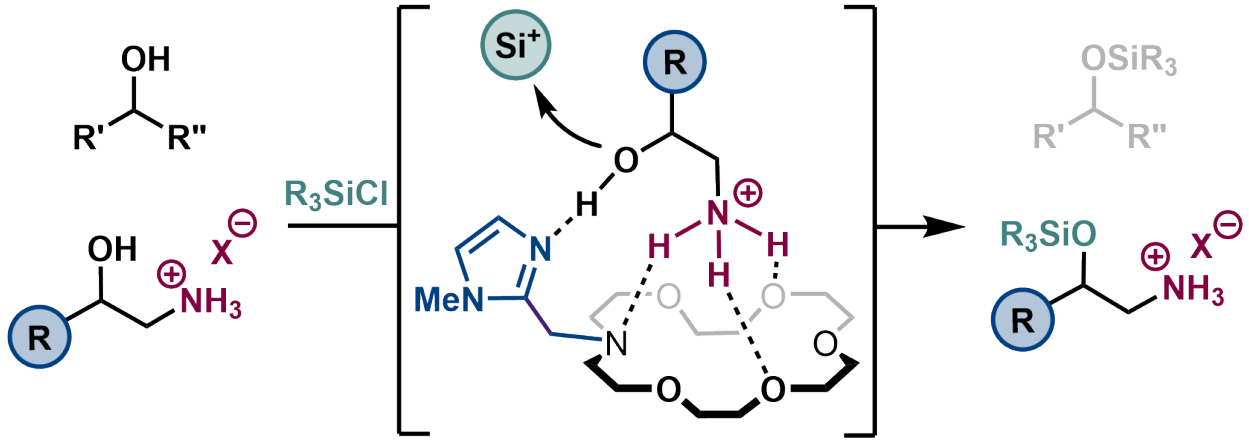
Proposed TS Structure
Enhanced reactivity of amines via weak noncovalent interactions

Polyamino systems are common in bioactive molecules, and selective modification of these motifs would provide a new avenue for drug discovery. Yet, catalytic site-selective functionalization of these polyamines remains underexplored due to the high the lack of catalytic methods and the inherent reactivity of aminesThe current state-of-the-art catalytic methods utilize nucleophilic catalysts, enzymes, or metal-catalyzed systems to undergo desymmetrization of meso and prochiral diamines. However, there is a limited scope of N-functionalization. There has yet to be a direct catalytic approach that enables diversification of amines. To address this challenge, we propose an alternative strategy to develop a new method that enhance the nucleophilicity of amine towards various electrophiles. This so-called, activation, strategy has been highly explored in the literature for O-functionalization of alcohols, but not with amines. Herein, we report a new strategy and catalyst design for the activation of amines using polyether catalysts as a H-bond acceptor. This poster will show our catalyst design for the rate acceleration of amines by using a simple N-arylation reaction as a model system. We observed optimal rate acceleration when we designed our catalyst to be a linear chain with flexible structural architecture. Based on these findings, we are currently developing a new chiral polyether catalyst for kinetic resolution of racemic amines.

Poster #4

Catalytic substrate-selective silylation and uranium binding studies using bifunctional macrocycles

Austin Seilkop, Kayleigh Wahr, and Boni Kim
Department of Chemistry



Recognition-driven, catalyst-controlled O-functionalization

In recent years, synthetic chemists have sought to create artificial catalysts that mimic enzymes, which can perform substrate-selective reactions in complex mixtures using multiple non-covalent interactions. However, substrate-selective catalysis remains less explored compared to chemo-, regio-, and enantio-selective catalysis. Taking this into consideration, our group aims to further develop the field of substrate-selective catalysis by designing catalytic methods that enable protecting group-free hydroxyl modification of amino alcohols. Performing selective amino alcohol functionalization faces two main limitations: the need for multi-step protecting group methods to achieve specific reactions, and the impediment of transition-metal catalysts due to strong binding with hydroxyl and amino groups. To address this challenge, we devised an alternative strategy by leveraging ammonium-recognition of crown ethers and multiple weak non-covalent interactions to enable substrate-selective functionalization of amino alcohols. Herein, we have developed a novel, bifunctional crown ether-based organocatalyst for the silylation of hydroxyl groups via ammonium-binding recognition-driven selectivity. Mechanistic studies based on substrate competition experiments show catalyst-controlled silylation of ammonium-alcohols over aliphatic alcohols, including natural products, up to >20:1 selectivity. In the future, we hope to use this strategy for peptides and complex aminoglycoside antibiotics. We can also extend the application of these macrocyclic compounds to bind radioactive metals such as uranium. By varying the electronic effects and pocket size on the macrocyclic ligands, we can further study the change in redox potential of uranium and the stability of the actinide complexes, respectively.

Poster #5

Upcycling mixed-material waste with elemental sulfur: applications to plant oil, unseparated biomass, and raw post-consumer food waste

Barbara G. S. Guinati, Perla Y. Sauceda Olono, Nawoda L. Kapuge Dona, Katelyn M. Derr, Shalini K. Wijeyatunga, and Andrew G. Tennyson and Rhett C. Smith
Clemson University

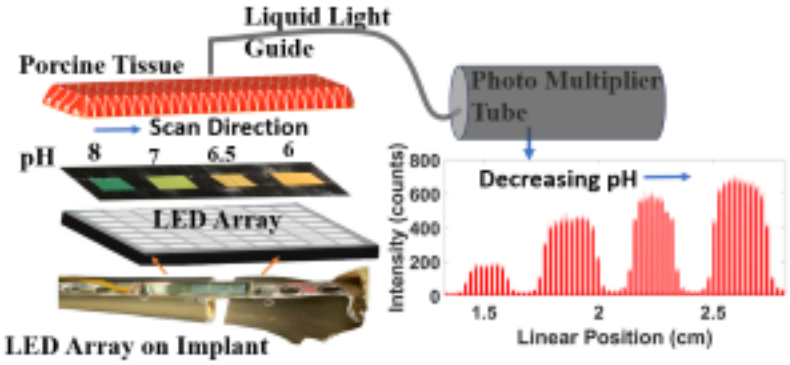
In this study, blends comprising triglycerides, unseparated biomass, and elemental sulfur that could be efficiently transformed into strong composites through the thiocracking method were investigated. Thus, a series of composites, HxOyS90, were prepared in which x = wt. % hulls, y = wt. % oil and sulfur composition was held constant at 90 wt. %.. Peanut hulls were mixed with elemental sulfur and peanut oil in a one-pot reactor to achieve strong composites. Aiming to broaden our investigation to encompass untreated post-consumer food waste, specifically French fries from a fast-food establishment, was used to prepare composites. Post-consumer French Fries were ground to produce small particles for reaction with sulfur (90 wt. %) at 180 oC for 24 h yielded composites WFFS90 that were incredibly strong materials with compressive strength 33.8 ± 0.3 MPa. Vacuum oven-dry French fries were also ground to yield even smaller particles for reaction with sulfur (90 wt. %) at 180 oC for 24 h yielded composites DFFS90. The proposed method poses exceptional outcomes by combining food waste, unseparated biomass and elemental sulfur. The materials prepared in this study are a potential alternative to ecologically harmful structure materials. Moreover, the insights provided contribute to valuable uses for food waste.

Poster #6

Micro-LED Display For Imaging Optical Absorption Targets Through Deep Tissue

Basanta Ghimire (1), Vigjna Abbaraju (2), Sriparna Bhattacharya (3), Herbert Belhow (4), Apparao Rao (5), and Jeffrey N. Anker (6)

(1)Graduate Student, Department of Physics and Astronomy, Clemson Nanomaterial Institute, Clemson University, (2)Graduate Student, Department of Chemistry, Clemson University, (3)Assistant Research Professor, Department of Physics and Astronomy, Clemson Nanomaterial Institute, Clemson University, (4)Research Associate, Department of Physics and Astronomy, Clemson Nanomaterial Institute, Clemson University, (5)Professor, Department of Physics and Astronomy, Clemson Nanomaterial Institute, Clemson University, (6)Professor, Chemistry and Bioengineering Departments, Clemson University



Imaging Through Tissue with Micro-Led Display

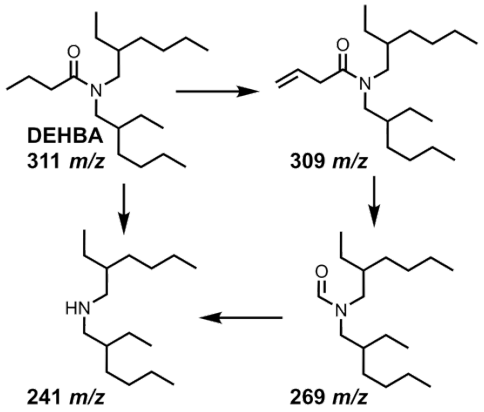
The presence of infection around implants can lead to localized acidosis, changing the pH levels due to bacterial activity and immune responses. Detecting these pH changes with high precision is crucial for early infection detection, treatment monitoring, and designing effective therapeutic techniques. This study focuses on the use of microlight-emitting diodes (OLEDs) for imaging pH variations around orthopedic implants within the body. OLEDs offer intense signals and cost-effectiveness. The research employs a flexible OLED display array as a local light source to assess the optical absorption of pH indicator dyes within tissues. By raster scanning light across different targets through varying thicknesses of porcine tissues (approximately 1-4 cm), the study captures the light passing through the tissues and optical reference targets using either a Nikon camera or a photomultiplier tube (PMT). The targets include a colored arrow printed on A4 paper and a pH reference strip. Successful reconstruction of the images of these targets demonstrates the color sensitivity and fine resolution achievable with this technique, primarily influenced by the pixel size of the OLEDs. Importantly, this approach enables imaging of different pH sensors even through tissues as thick as ~4 cm. Overall, these findings emphasize the potential of OLEDs for non-invasive and effective imaging of local optical absorption targets including pH indicators on implanted medical devices to study local pH near the device surface during implant-associated infections.

Poster #7

Establishing Correspondence Between Radiolytic and Non-Radiolytic Radical Degradation of Monoamide Extractants

Brandon G. Wackerle (a), Madison R. Vicente (a), Dean R. Peterman (b), Modi Wetzler (a), and Julia L. Brumaghim (a)

(a) Department of Chemistry, Clemson University, Clemson, SC 29634-0973, (b) Aqueous Separations and Radiochemistry, Idaho National Laboratory, Idaho Falls, ID 83415-6158



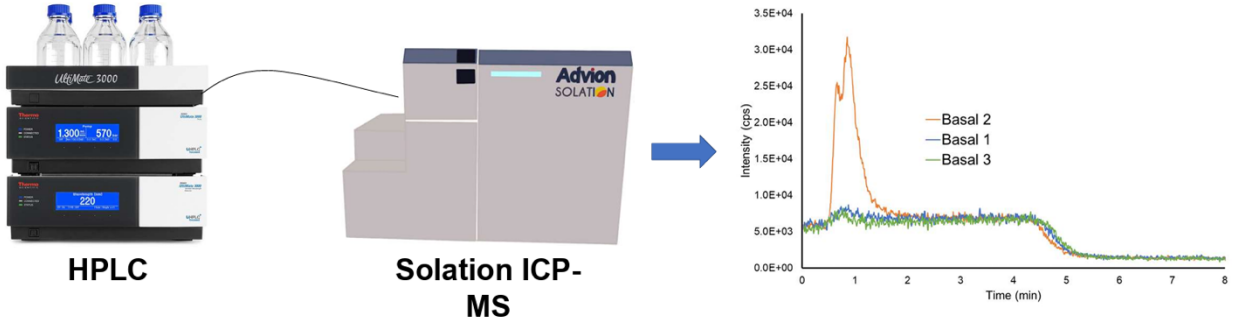
Dialkyl amides such as N,N-di-2-ethylhexyl-isobutyramide (DEHiBA) and N,N-di-2-ethylhexyl-butyramide (DEHBA) have been studied as alternatives to tributyl phosphate (TBP). The PUERX (Pu and U Reduction Extraction) process uses TBP as the extractant to recover Pu and U from nuclear waste, but waste incineration is difficult due to the presence of phosphorus and the formation of a third-phase can occur. Alternatively, monoamides are more readily incinerable than TBP and their carboxylic acid and amine degradation products prevent third-phase formation because of their water-solubility. Although monoamides are promising extractants, they must also be radiolytically stable to allow for scale-up of the separation process. Gamma-radiolysis is the gold standard to study the effects of radiation on materials, but is a low-throughput process which has limited researchers ability to broadly study the radiolytic stability of monoamides, making it difficult to conclude what effects alkyl branching has on the complexant stability. Thus a higher throughput method of predicting the radiolytic stability of novel complexants and identifying key targets for further study via gamma radiolysis is required. We are developing a non-radioactive radical assay as a potential screening tool to help alleviate the bottleneck of traditional, but high-cost gamma radiolysis studies. Azohydroperoxide forms hydroxyl radical and *tert*-butyl radical upon heating in toluene as the organic solvent, which is necessary due to the insolubility of monoamide complexants in water. Using gas chromatography mass spectrometry (GC-MS) to analyze these radical assays, we have identified the same degradation products, including amine, secondary amide, amide and solvent-adduct products, are formed in the radical assay and gamma radiolysis of the monoamides in toluene. Additionally, bibenzyl resulting from the termination of two toluene radicals is observed in the GC-MS. This observation allows us to determine the amount of bibenzyl produced as a function of absorbed dose from gamma radiolysis and the concentration of

azohydroperoxide added in the radical assay. The dose response for the formation of bibenzyl allows us to establish a correspondence between the two methodologies and semi-quantitatively predict the radiolytic stability of these monoamide complexants. Analysis of the irradiated DEHBA and DEHiBA samples via GC-flame ionization detection (FID) have shown agreement to literature, indicating similar dose dependance in toluene. Overall, results are indicating a promising ability for radical assays to be used as a screening tool to quickly examine the radiolytic stability of monoamide complexants prior to more in-depth gamma radiolytic studies. We have started targeting other monoamides with varying N and C branching to identify how structure impacts stability.

Poster #8

Comprehensive Mass Metals Balance in CHO Cell Processes

Cameron Stouffer 1, Sarah Wysor 1, and R. Kenneth Marcus 1
(2) Department of Chemistry, Clemson University



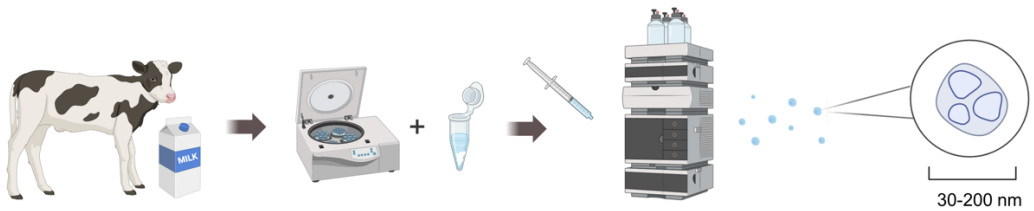
HPLC **Solation ICP-MS**

It is well established that the metal content in Chinese hamster ovary (CHO) cell culture media (CCM) significantly affects process productivity and critical quality attributes (CQAs). Metals exist in diverse chemical forms in CCM, which may change during the monoclonal antibody (mAb) production cycle. Naturally, it is postulated that the chemical speciation of these metals affects their uptake and metabolism. While the targeted forms of metals in media are company-specified, their commercial sources, as well as those of the organic media constituents, may result in concentrations and speciation that differ from the intended formulas. Therefore, there is a need for a method to determine the concentration of metals and their chemical forms. Presented here is a methodology to speciate inorganic-versus-ligated metals using high-performance liquid chromatography (HPLC) employing a polypropylene capillary-channeled (C-CP) fiber column with inductively coupled plasma mass spectrometry (ICP-MS) determinations of five target metals (Mn, Fe, Co, Cu, and Zn). A 50 µL injection of CCM supernatant is used for an effective quantification method to identify metal speciation and concentration deviations from reported formula levels. Two case studies as to the utility of the methodology are presented: shelf-life and chemical contamination. The further development of this method will allow for improvement in quality control, identification of contaminants, assessment of media stability/degradation products, and measurement of whole cell metal uptake in these growth media.

Poster #9

Milking It: Isolation of Bovine Milk Derived Extracellular Vesicles via a Capillary Channeled Polymer (C-CP) Fiber Stationary Phase

Carolina Mata (1) Jerisa Pimentel (1), and R. Kenneth Marcus (1)
(1) Department of Chemistry, Clemson University



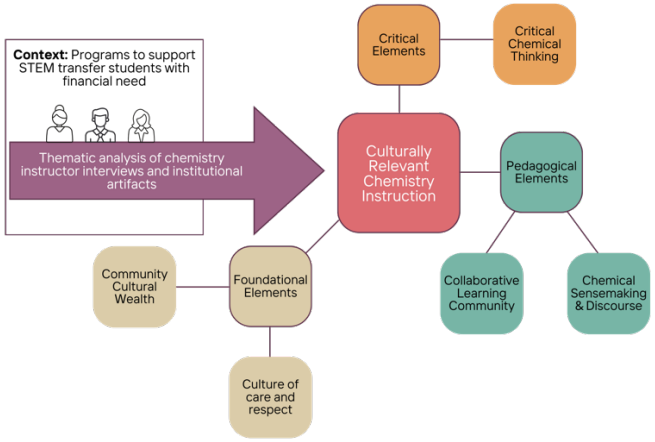
Extracellular vesicles (EVs), which are excreted from most cell types are membrane-bound vesicles ranging in size from 30-200 nm. EVs, also known as exosomes, serve as transportation vehicles for biomolecules and biomarkers in cellular communication pathways. Exosomes have captured the interest of the biomedical community for their potential in biomarker detection and therapeutics due to their biocompatibility and ability to transport information from cell to cell. Isolation of exosomes from mammalian cells has posed challenges in the field due to cost, extended analysis time, impure yields, lack of biocompatibility, and accessibility. Current, size-based methods of exosome isolation including ultracentrifugation and size exclusion chromatography are not immune to these challenges, prompting the need for a more efficient separation method. Exosomes from bovine milk are of interest due to their broad availability and non-toxic characteristics making them a promising, cost effective source for therapeutic applications. Current challenges in the isolation of milk derived extracellular vesicles (MDEVs) are posed by heavy matrix effects. Fats and proteins in particular have added an extra layer of complexity to the isolation of MDEVs. Casein, a protein abundant in milk, forms micelles with similar characteristics to EVs including function, stability, and size range. Their similar characteristics make it difficult to separate the two entities based solely on size and density. However, by pre-treating bovine milk with acetic acid to precipitate the casein micelles and excess proteins, a capillary channeled polymer (C-CP) fiber phase in a column format can be applied to alleviate these challenges. The C-CP fiber column enables the separation of MDEVs from treated milk based on hydrophobicity, where a stepwise gradient ensures small molecules are unretained under high salt, proteins are released by lowering the salt content, and EVs are eluted using an organic solvent. Using C-CP columns to isolate MDEVs is cost and time effective, with a price tag of less than $5 per reusable column and an isolation time of less than 12 minutes with yields up to particles/mL. The integrity of the vesicles post isolation was verified using transmission electron microscopy (TEM), nanoparticle flow cytometry (NanoFCM), and bioassays. This low cost and efficient isolation method holds significant promise for the use of MDEVs in downstream therapeutic applications.

Authors acknowledge the financial support from NSF, Division of Chemistry, award CHE-2050042 (REU Program)

Poster #10

Elements of culturally relevant instruction: An instructional framework for college chemistry instructors

Destinee Cooper (1), and Dr. Matthew Voigt (1)
(1) Clemson University

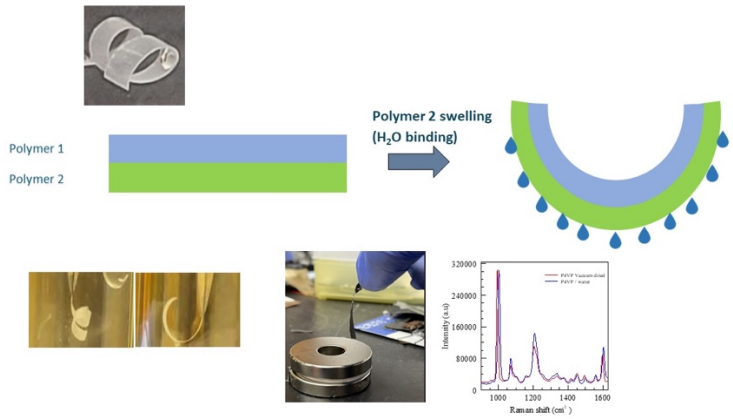


Implementing pedagogical practices that center students and their strengths is necessary to realize the goal of equitable and effective chemistry instruction. Asset-based teaching approaches have been shown to foster learning environments that promote students,Äô success and holistic well-being across a variety of disciplines and academic levels. Culturally relevant pedagogy (CRP) is one asset-based framework designed to support instructors in elevating students, strengths and backgrounds to inform classroom norms, practices, and instruction. We believe that chemistry instructors,Äô adoption of CRP will support chemistry students, understanding of disciplinary core ideas and engagement in science practices. However, college chemistry instructors, knowledge and implementation of culturally relevant instructional practices have not been widely studied. This exploratory study examines how college chemistry instructors at both associate's and bachelor's degree-granting institutions in the United States describe and operationalize culturally relevant pedagogy in general and organic chemistry courses. The faculty participants (N=3) were purposively sampled for their expressed interest in CRP and their departmental affiliation with a program to support low-income transfer students in chemistry. Thematic analysis of semi-structured instructor interviews and institutional artifacts reveal key constructs that are important for culturally relevant chemistry instruction: flexibility in teaching and curriculum, cultivating a community of collaboration and belonging, and affirming that all students have the intellectual capacity to be successful in chemistry. These practices are foundational elements of culturally relevant chemistry instruction, but they must also be coupled with knowledge of students, cultural wealth and awareness of sociopolitical issues that impact students. We developed an instructional framework that builds on the original tenets of CRP to support college chemistry instructors, understanding and implementation of culturally relevant chemistry instruction. Future work will examine the use of our framework for chemistry faculty development.

Poster #11

Stimuli-Responsive Self-Folding Polymer Bilayer Films

Dimuthu Edirisinghe (1), Astrid Garcia (1), and George Chumanov (1)
Department of Chemistry, Clemson University



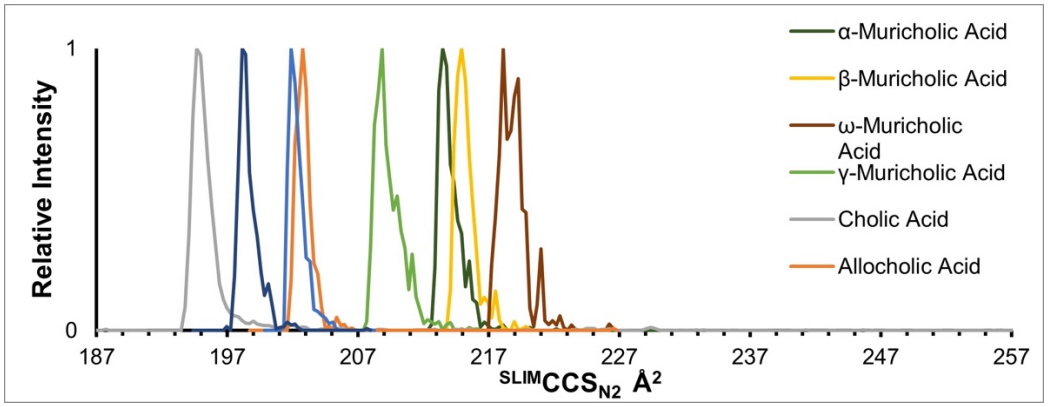
The development of stimuli-responsive, self-folding materials is important in designing various smart functional materials and actuators. Material self-folding is referred to as the initial structure folding into different shapes such as curves, spirals or other three dimensional structures either spontaneously or as a response to a stimulus without any active human control. The use of soft materials for developing applications for actuation is the modernized way as it gives a relatively large number of degrees of freedom compared with hard materials. Soft actuating materials often employ polymers due to their unique mechanical and chemical properties that can be modified to obtain sensitivity toward a broad range of stimuli. Well-adhered polymer bilayers are an interesting approach to designing self-folding structures. One polymer layer should be inactive or comparatively less active toward the particular stimulus to obtain the reversible folding and unfolding caused by swelling/dwelling or expansion/shrinking of the one polymer layer compared to the other one. The development of reversible self-folding polymer bilayers that are sensitive to chemical changes in the environment is presented in this project.

*Authors acknowledge the financial support from NSF, Division of Chemistry, award CHE-2050042 (REU Program)

Poster #12

High-Resolution Ion Mobility Analysis of Isomeric Bile Acids Using Structures for Lossless Ion Manipulations (SLIM) IM-MS

Emmaleigh Efird (1), Makenna Hoover (1), Terra Pettit-Bacovin (1), Ashlee Wedge (1), and Christopher D. Chouinard (1)
Department of Chemistry



Bile acids are an essential part of the human digestion system and play an important role in lipid absorption, bacteria movement in the small intestine, and regulation of the FXR and TGR5 receptors responsible for homeostasis. Gastritis and diabetes are examples of diseases linked to bile acid metabolism, making their identification important for biomedical applications and clinical diagnostics. While this has historically been performed using chromatographic and/or mass spectrometric methods, the ability to rapidly differentiate bile acid isomers remains a critical need. In this study, we use high-resolution Structures for Lossless Ion Manipulations (SLIM) ion mobility (IM) to optimize bile acid separations and measure collision cross section (CCS). Data was acquired in full-resolution and data dependent MS/MS (DDA) modes using nitrogen or helium gas, for comparison of mobility resolution and sensitivity. All data was processed using the PNNL PreProcessor and Agilent IM-MS Browser 10.0. SLIM CCS values were calculated based on calibration using either the Agilent Tune Mix ions or a subset of bile acid calibrants, for comparison with their *true* values measured with the drift tube IM-MS. We further investigate the potential for using this approach in quantitative clinical applications.

Poster #13

Synergistic Antioxidant Enhancement via Functional Deep Eutectic Systems

Emmanuel D. Dike (a), Lucas B. Ayres (a), Tomas E. Benavidez(a), Jorge Barroso Moreno (a), and Carlos D. Garcia (a)
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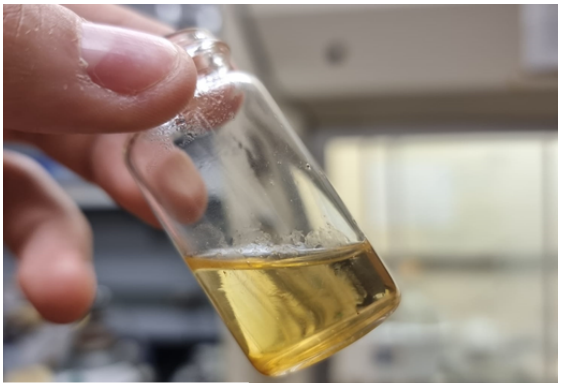
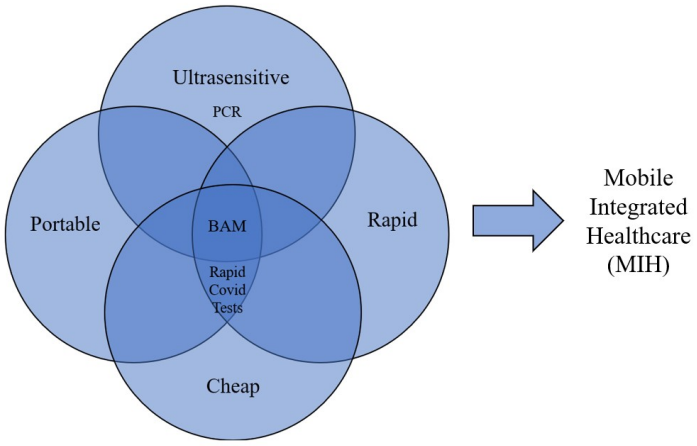


The degradation of unsaturated lipids in food products leading to the formation of potentially harmful reaction by-products, that cause a change in color, flavor and odor (rancidity) in food products is a major food health challenge. Among several strategies to mitigate the adverse effects of rancidity, the use of antioxidants has shown impeccable efficiency inhibiting these oxidative processes in food, there by preserving quality and shelf life. It is important to point out that the complicate interplay between antioxidant mixtures results in different antioxidative effects (synergistic effects, antagonistic effect and additive effect). Among these interactions, it has been confirmed that synergism is one of the most effective in improving oxidative stability. In this context, our group explored the use of artificial intelligence to develop a model capable of predicting combinatorial indexes of synergistic antioxidants. In parallel to this development, our group has also deployed the use of advanced AI models to grasp the complexity and understand the intricate interactions of eutectic mixtures such as deep eutectic solvents (DES). The developed algorithm from this particular research was capable of predicting the melting point of these mixtures at specific molar ratios. Based on these two researches, we discovered that commonly used synergistic antioxidants can be effectively deployed in the formulation of deep eutectic solvents (DES) that remain stable at room temperature. This remarkable discovery could leverage the enhancement of synergistic antioxidants in DES form, which this particular study addresses. The aim of this study was to investigate the antioxidative activities of the first-ever DES formulated with synergistic antioxidants, butyl hydroxyanisole (BHA) and butylated hydroxytoluene (BHT) on the basis of thiobarbituric acid reactive substances (TBARS) in cow and olive oil fats. The results from this assay showed that the DES exhibited higher antioxidative capacity compared to the BHA-BHT synergistic mixture.

Poster #14

The Application of Buoyant and Magnetic (BAM) Assays for Detecting Individual SARS-COV-2 Nucleocapsid Proteins for Mobile Integrated Healthcare (MIH)

Emory Satterfield (a), Jade Johnson (a), and Zahra Karimpour (a), Chuanlei Wang (a), Dr. Jeffrey N. Anker (a)
(a) Department of Chemistry



We are developing a rapid screening test that can detect the presence and concentration of SARS-CoV-2 in a patient's saliva using buoyant and magnetic microbeads. These microbeads are functionalized with antibodies targeting and binding to the SARS-CoV-2 nucleocapsid protein in a patient's saliva, forming buoyant-and-magnetic (BAM) complexes. The BAM complex consists of a buoyant microbead and a magnetic microbead bound to a single viral protein through antibodies. The naked eye can see these BAM complexes, but video analysis through MATLAB has allowed us to track the individual motion of the individual BAM complexes. We are currently optimizing the assay by creating ways to separate the beads by size, analyzing the effects of bead size on assay performance and reproducibility, and analyzing the binding probability altered through the various bead sizes. We are designing and 3D-printing stands to allow us to conduct multiple trials in parallel. Once optimized, this test has many applications within the mobile integrated healthcare (MIH) field. Within the MIH field, this test can deliver on-site results within 15 minutes without any complex equipment, providing a robust and quickly executable point-of-care test for COVID-19.

Poster #15

Supramolecular œÄ-Donor/Acceptor Arrays Based on Inclusion Complexes of Zn-Porphyrin Cages and Intercalated œÄ-Acceptor Guests

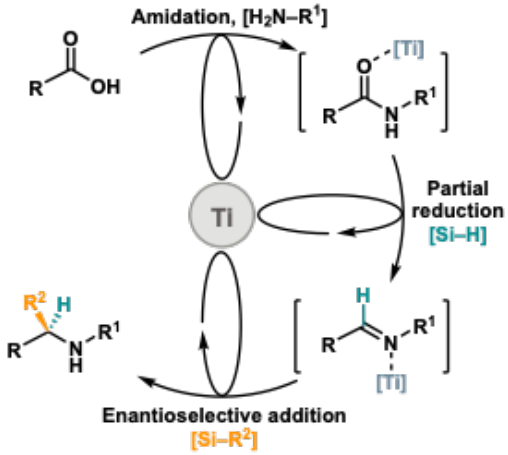
Evan Thibodeaux, Paola A. Benavides, Monica A. Gordillo, Ashok Yadav, Evan Johnson, Rakesh Sachdeva, and Sourav Saha
Department of Chemistry

In recently published work we demonstrated that a tetragonal prismatic metal-organic cage ($MOC1^{8+}$) having two parallel π-donor tetrakis(4-carboxyphenyl)-Zn-porphyrin (ZnTCPP) faces selectively intercalate planar π-acceptor guests, such as hexaazatriphenylene hexacarbonitrile (HATHCN), hexacyanotriphenylene (HCTP) and napthalenediimide (NDI) derivatives, forming 1:1 πA@$MOC1^{8+}$ inclusion complexes featuring supramolecular π-D/A/D triads. The π-acidity of intercalated π-acceptors (HATHCN ≫ HCTP ≈ NDIs) dictated the nature and strength of their interactions with the ZnTCPP faces, which in turn influenced the binding affinities (K_a) and optical and electronic properties of corresponding πA@$MOC1^{8+}$ inclusion complexes. Owing to its strongest CT interaction with ZnTCPP faces, the most π-acidic HATHCN guest enjoyed the largest K_a (5×10^6 M^{-1}) competitively displaced weaker π-acceptors from the $MOC1^{8+}$cavity and generated the highest electrical conductivity (2.1×10^{-6} S/m) among the πA@$MOC1^{8+}$ inclusion complexes. These inclusion complexes exhibited unique through-space charge transport capability which generates tunable electrical conductivity, a rare and coveted electronic property of supramolecular assemblies that could lead to utility in future technologies. Expanding further upon this work, the larger cage $MOC2^{8+}$ was selected to in order to accommodate up to three guest molecules and form [D·A/D'/A·D]-type inclusion complexes that benefit from D/A CT interactions between the ligands and guests, as well as the D/A interaction between the guest molecules. These larger inclusion complexes should exhibit greater charge delocalization and therefore even greater conductivity than the triads of $MOC1^{8+}$. Additionally, after assembling the inclusion complexes and assessing their properties, we plan to assemble daisy chain coordination polymers (DCCPs) by tethering the cages with exo-axially coordinated linear dipyridyl linkers, the length of which should be dependent on the ratio between cage and linker. These DCCPs should also further increase charge delocalization for these materials.

Poster #16

Titanium-Based Multicatalysis: Accelerated Enantioselective Synthesis of Chiral Amines

Giovani Gutierrez (1), Jason Wilt (1), Samirah Muhammad (1) Diego Rodriguez (1), Emily Girotti (1), and Byoungmoo Kim (1)
(1) Department of Chemistry, Clemson University



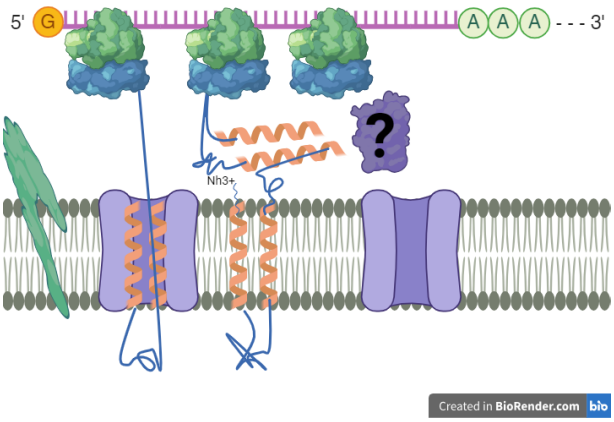
Inspired by the efficiency of enzymatic systems that occur in nature, the field of multicatalysis has emerged as a powerful synthetic strategy that enables access to unprecedented transformations. Multicatalytic processes combine numerous catalytic reactions in a ‚Äúone-pot‚Äù fashion, which reduces reaction time, chemical waste, and cost. Herein, we present our recent developments in the Kim Group, where we developed a novel multicatalytic system that combines simple amine and carboxylic acid building blocks to furnish enantio-enriched chiral amines. Our multicatalytic system employs a single, readily available titanium catalyst that can facilitate three distinct catalytic transformations under a mild condition: 1) direct coupling between a carboxylic acid and a primary amine to generate an amide intermediate, 2) selective partial reduction of the amides to imines, and 3) enantioselective cyanation of imines to generate chiral amine products up to 90% ee. Our methodology has demonstrated high functional group tolerance and applications towards diversifications of pharmaceutical relevant compounds.

Authors acknowledge the financial support from NSF, Division of Chemistry, award CHE-2050042 (REU Program)

Poster #17

Proposed Chaperone Protein Involved in Synthesis of Type IV Transmembrane Proteins

Harry Kish (a), Tsaddiyq Morbeth (a), and Soren Spina (b)
(a) Department of Biological Sciences, Clemson University (b) Department of Genetics and Biochemistry, Clemson University

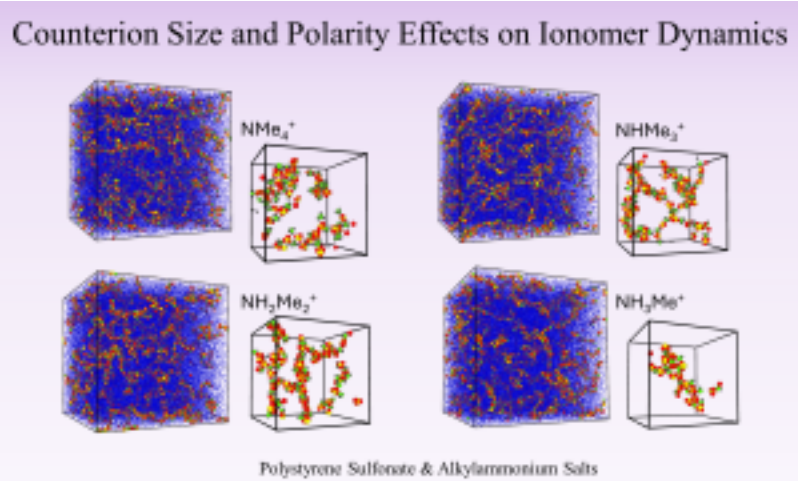


For the Synthesis/Translocation of Type IV (GLUT1), a mRNA holds a ribosome carrying a secretory protein with a positive charge in the cytosol having an internal anchor sequence. The SRP (Signal Recognition Particle) will bind to the internal anchor sequence, leading the signal peptide to the SRP Alpha beta receptor on the endoplasmic reticulum. Once bonded, GTP hydrolysis will be enacted and the translocon gate will be opened, allowing the ribosome to insert the first integral signal and stop-transfer sequence. Once inserted, it will diffuse out of the translocon into the membrane, keeping the receptor in place. Then, the ribosome will synthesize the nascent protein into the cytosol. The mechanism to keep these sequences from unfolding is unknown. These sequences consist of anchor and stop transfer signals to be inserted into the translocon and diffused outward into the membrane. The process will continue until 12 helices have been placed in the ER for (GLUT1). The C-terminus will also have hydrophilic amino acids near the hydrophobic sequence, allowing it to be located in the Cytosol. Here, we propose a protein that could stabilize the following anchor and stop transfer signals in the cytosol. The abstract figure was created with BioRender.com.

Poster #18

Counterion Size and Polarity Effects on Ionomer Dynamics

Hayden Sasko (a), Chathurika Kosgallana (a), Gary Grest (b), and Dvora Perahia (a)(c)
(a) Department of Chemistry, (b) Sandia National Laboratory, (c) Department of Physics



Numerous studies have shown that clustering of ionizable polymers controls the structure and dynamics of these macromolecules and consequently affects their properties. The clustering process is impacted by several factors, among them polymer topology and electrostatic interactions. With the goal of understanding the interrelation between clustering and polymer dynamics, the current study uses atomistic molecular dynamics (MD) simulations to probe the effects of counterion size and polarity on the dynamics of polymer melts using polystyrene sulfonate in the ionomer regime with sulfonation fraction f=0.09, below its entanglement length. The counterion chosen is NR4+ with R=H or CH3 , varying the ratio of CH3:H affecting the size and the polarity of the cation. The systems were built in BIOVIA, Molecular Studio, and ran in LAMMPS and GROMACS. The static and dynamic structure factors were calculated and correlated with the characteristics of the ionic clusters. We find that this series of counterions significantly modifies the cluster size and shape in comparison to small inorganic cations such as Na+, impacting the structure and dynamics of the melts. The structure of the melts as the counterion is varied will be first discussed followed by introducing the dynamic structure factor S(q,t) and mean square displacement studies that together capture the motion of the polymers on multiple length scales.

Poster #19

Imidazole Thiones Show Metal-Mediated DNA Interactions

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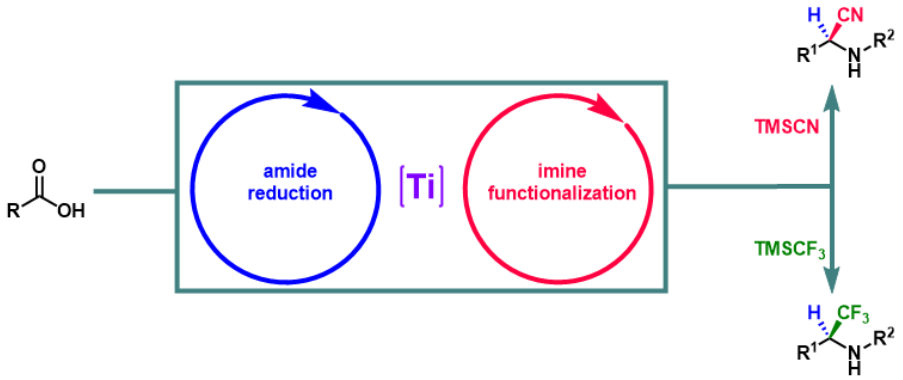
(a) Department of Chemistry, Clemson University

Sulfur-containing imidazole thiones are widely studied as antioxidants, and the antithyroid thione-containing drug methimazole (N-methyl imidazole) is reported to weakly localize on DNA as determined by UV-vis and circular dichroism (CD) spectroscopies. In our hands, isothermal titration calorimetry (ITC) and CD titrations indicate no methimazole-DNA interactions up to 100 ¬µM methimazole titrated into 100 µM DNA base pairs. A related compound N,N-dimethyl imidazole thione (dmit) also shows no DNA localization using these methods. In contrast, when dmit and Fe(II) are added to DNA, Fe(II) mediates a helicity-perturbing interaction that is not present in DNA titrations of either dmit or Fe(II) alone. Both Fe(II) and Zn(II) ions show similar DNA interactions in CD titrations, and both metal ions are known to localize on DNA bases and the phosphate backbone. Thus, Zn(II) was used to mimic Fe(II) in ITC titrations to avoid iron oxidation and precipitation. Zn(II) binding to DNA is spontaneous (□ΔG = -6.9 kcal/mol) with a maximum stoichiometry of 0.59 ± 0.02 Zn(II) ions per base and a Kd value of 9 ± 2 ŒºM. When the thione-metal complexes Zn(dmit)2Cl2 is titrated into DNA, an increase in the CD helicity band (245 nm) and a decrease in the base-stacking band (275 nm) are observed, and ITC data show that Zn(dmit)2Cl2 likely interacts more strongly with DNA than Zn(II) alone. These data indicate that metal ions can control small-molecule-DNA interactions and that ternary antioxidant-metal-DNA interactions may be a novel mechanism by which antioxidants prevent metal-mediated oxidative DNA damage.

Poster #20

Titanium-Multicatalytic Diversification of Amides

Jason Wilt, Giovani Gutierrez, Samirah Muhammad, Diego Rodriguez, and Byoungmoo Kim
Department of Chemistry, Clemson University



Amides are one of the prevailing functional motifs in biomolecules, making them a highly attractive synthetic motif for drug diversification. However, due to their chemical stability, harsh reagents with poor functional group tolerance compatibility are often implemented for amide diversification. In response to address this gap, transition-metal catalyzed hydrosilylation has provided selective and mild methodologies toward amide reductive transformations. Noble metals possess high hydrosilylation activity at very low catalyst loadings, particularly iridium, ruthenium, and rhodium. However, noble metals are rare and expensive, which creates incentive to develop systems using earth-abundant metals. Also, the current enantioselective methods for amide diversification require two separate catalysts, one for reduction and the other for functionalization, which is wasteful. Here, we present the use of an earth-abundant titanium for enantioselective amide diversification via sequential partial amide reduction and enantioselective imine functionalization. We also demonstrated that our titanium catalyst could perform direct amidation on carboxylic acids and simple amines in situ, enabling three successive synthetic steps to be performed with the same catalyst. Using TMSCN as a model nucleophile and an inexpensive chiral aminoalcohol ligand, the desired aminonitrile products were obtained up to 96% ee. We are currently expanding the scope of this multicatalytic system to incorporate fluoroalkyl groups, which are attractive motifs in medicinal chemistry due to their ability to increase compound lipophilicity and alter active conformation.

Authors acknowledge the financial support from NSF, Division of Chemistry, award CHE-2050042 (REU Program)

Poster #21

Uranium Isotope Ratios Directly from Environmental Swipe Surfaces Using the Liquid Sampling, Atmospheric Pressure Glow Discharge Ion Source Coupled with an Orbitrap Mass Spectrometer

Joseph V. Goodwin 1, Benjamin T. Manard 2, Brian W. Ticknor 2, Paula Cable-Dunlap 3, and R. Kenneth Marcus 1

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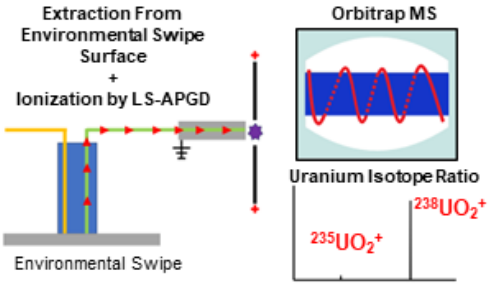
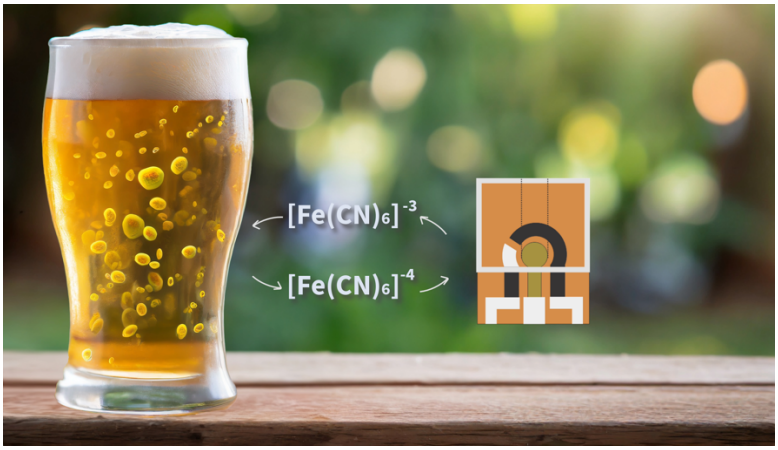


Environmental swipes are a powerful investigative tool the nuclear safeguarding community uses to verify states' declarations to international regulatory agencies. Determining uranium isotope ratios from environmental swipes provides investigators with information on types of processing and levels of uranium enrichment used within the investigated facility. Traditional methods of processing environmental swipes are complex and time-consuming, requiring numerous ashing and extraction steps before an isotope ratio measurement is made. In addition, the isotope ratio typically reported from environmental swipes is a "bulk average," or the average isotope ratio found for all particles of uranium contained on the swipe. Since a bulk average is reported, it is possible for the result to obscure the presence of higher enrichment uranium particles by more abundant uranium particles with a lower enrichment level or even natural uranium present in the cotton used to make the environmental swipe. To provide investigators with rapid results as well as spatial resolution of the environmental swipe surface, a microextraction technique initially developed for extractions from TLC plates has been adapted for measuring uranium isotope ratios directly from the environmental swipe surface. Briefly, the uranium present on the swipe surface is mobilized and directed to the liquid sampling ‚Äì atmospheric pressure glow discharge, a novel microplasma ionization source, which has been coupled with the ultra-high resolution Orbitrap mass spectrometer. This results in a relatively compact, forward-deployable analytical platform that can report results with spatial resolution from environmental swipes that are unbiased by natural uranium in the environmental swipe. The results of this study show that uranium isotope ratios obtained by the microextraction procedure more closely match the known isotope ratio (~100% of known) of the standard used than the isotope ratio determined by the traditional bulk average method (~75% of known).

Poster #22

How active are the microorganisms in your yogurt? New cardboard sensor to study probiotic activity

Juliana L. M. Gongoni (a), George Chumanov (b), Thiago R. L. C. Paix√£o (a), and Carlos D Garcia (b)
(a) University of Sao Paulo (Brazil), (b) Clemson University

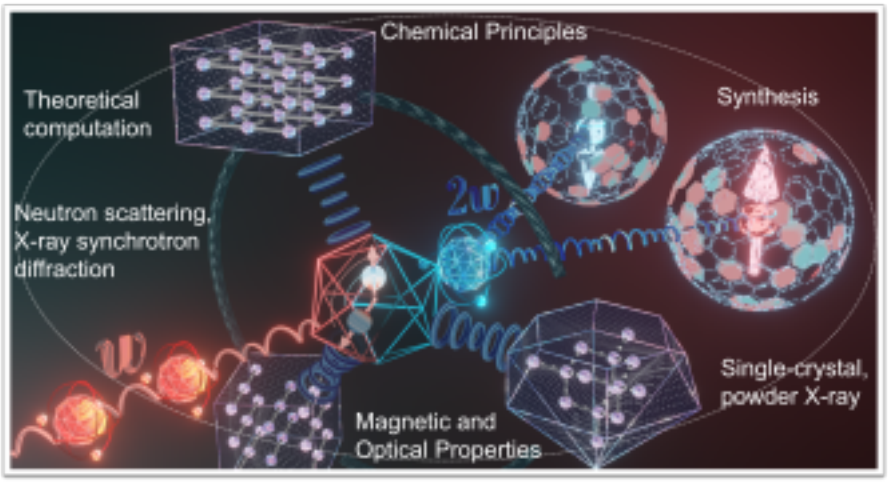


A simple and fast (<15 min), two-step laser scribing of cardboard substrates is described as a method for fabricating carbon electrodes modified with metallic nanoparticles. The first scribing step patterned a cardboard substrate (promoting the formation of porous carbon electrodes). The second step was included to produce metallic nanoparticles via a chemical reduction process of cations from an aqueous solution. For these experiments, the effects of copper, silver, nickel, cobalt, zinc, and gold were evaluated considering their effect on the electrical properties and the composition of the carbon materials produced. These experiments revealed that, despite significant changes in resistance (from 138±7 Ω for plain electrodes to just 53±3 Ω for Au-modified electrodes), only marginal changes were observed in the morphology or composition of the material produced (I_G/I_D ranged from 1.2±0.3 for the plain cardboard to 1.8±0.3 for the cobalt-modified electrodes). To demonstrate the applicability of the proposed strategy, Au-modified electrodes were assembled into electrochemical sensors and applied to measure the metabolic activity of live microorganisms in various commercial samples, requiring only 100 µL of sample and 10 min of incubation time.

Poster #23

Addressing Fundamental Challenges in Energy and Information Science and Technology through Materials Chemistry

Kayla Lea, Matthew Caimbeul, Athira Babu, Keegan Hommerding, Uchenna V. Chinaegbomkpa, Dasuni N. Rathnaweera, Xudong Huai., and Thao T. Tran
Department of Chemistry, Clemson University, SC 29634, USA



If only we could unlock the potentials of quantum and functional materials that are the basis of advanced memory and computational platforms by tuning their structure and behavior, we could revolutionize energy and information science and technologies and transform our world. While this cross-disciplinary research is critical in enabling pathways to foreseeable technologies, a significant challenge in the field has been poor control over structural and electronic modification under the strict constraints required for manipulating spin dynamics by external stimuli. To address this challenge, our team seeks to understand materials at the atomic level and harness chemical bonding and electronic structure to develop quantum and functional materials with targeted properties. Examples include optically addressable magnets, topologically nontrivial spin systems, and materials with strong quantum fluctuations. In this poster, we will highlight a set of tools and thinking processes we use to design, create, and characterize quantum and functional materials. We will discuss a few examples of our work and how we apply chemical logic to understand and develop materials directly relevant to energy and information technology research.

Poster #24

Halogen Bonding in Cocrystals of Organoiodines with Diphenyliodonium Chloride/Iodide Salts

Lahiruni Pelendage, Colin McMillen*, and Dr. William Pennington
Department of Chemistry, Clemson University

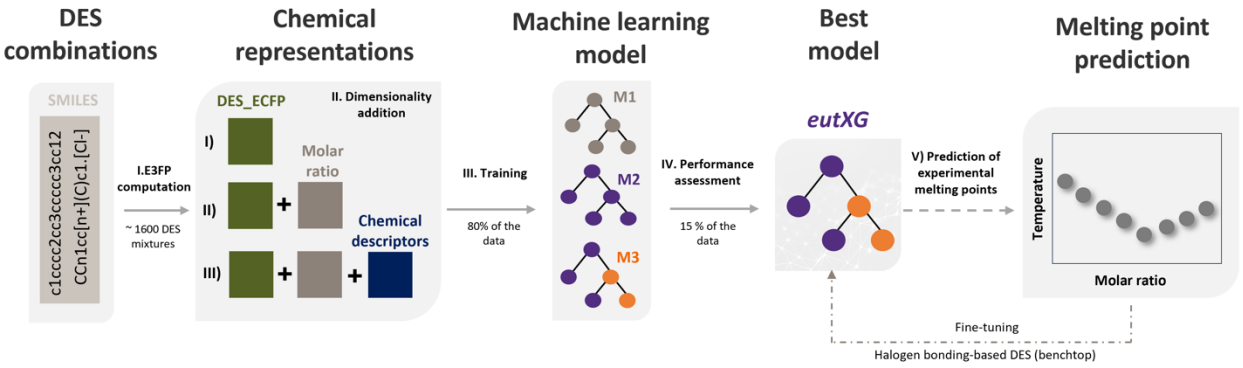
A series of novel halogen bonded cocrystals of diphenyliodonium iodide (DPhII) and diphenyliodonium chloride (DPhICl) with the organoiodines: 1,2-diiodotetrafluorobenzene (1,2-F4DIB), 1,3-diiodotetrafluorobenzene (1,3-F4DIB) and 1,4-diiodotetrafluorobenzene (1,4-F4DIB) are reported. Cocrystals obtained by solution synthesis and mechanochemical synthesis are compared. The assembled cocrystals were studied by X-ray diffraction and powder X-ray Diffraction (PXRD) to evaluate the structures. Interestingly, the chloride and iodide systems often demonstrate differing behavior, either through the formation of different cocrystalline ratios, or through the formation of non-isostructural assemblies. A key feature of the structures is the formation of a rhombus-like halogen bonding core between the cations and anions in the cocrystal structures. The organoiodines are appended to this core in various ways, depending on the organoiodine isomer involved, and the cocrystal ratio. This study compares structural features such as the halogen bonding strength (distance) and long-range halogen bonding patterns involving the iodide and chloride anions. More broadly, the study develops the rhombic halogen bonding motif to develop reliable crystal engineering principles.

Poster #25

eutXG: A Gradient Boosting Model to Predict the Melting Point of Deep Eutectic Solvents

Lucas B. Ayres (a), Madushi Bandara (a), Collin D. McMillen (a), William T. Pennington (a), and Carlos D. Garcia (a)

(a) Department of Chemistry, Clemson University

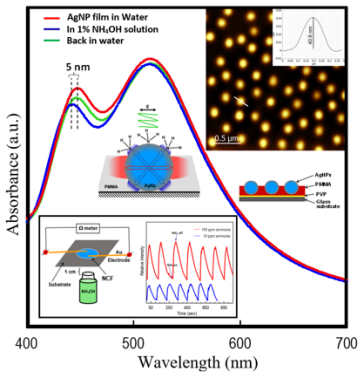


We present the application of an extreme gradient boosting model to predict the melting point of deep eutectic solvents (*eutXG*). The model is based on XGBoost, a decision tree ensemble based on gradient boosting designed to be highly scalable, that enables superior training speed and prediction accuracy. The selected model – trained with molecular fingerprints, molar ratios, and selected chemical descriptors– enabled predicting the melting points of DES with an average accuracy of 97.6%, which represents, on average, a difference of just 12 K with respect to the values reported in the literature. Using Shapley Additive exPlanations (SHAP), further insights into the relative importance of different inputs used to train the machine learning model were identified. Moreover, the generalization ability of the *eutXG* model was critically assessed by comparing the predicted vs the experimentally-determined melting point of a series of novel DES based on halogen bonding, developed by mixing tetrahexylammonium triiodide ($NHex_4I_3$) and 1,2-diiodotetrafluorobenzene (oF_4DIB) in various molar ratios.

Poster #26

Silver nanoparticle composite films for sensing ammonia in the presence of water vapor

Madhuka Liyanage (a), Robert Latour (b), and George Chumanov (a)
(a) Department of Chemistry



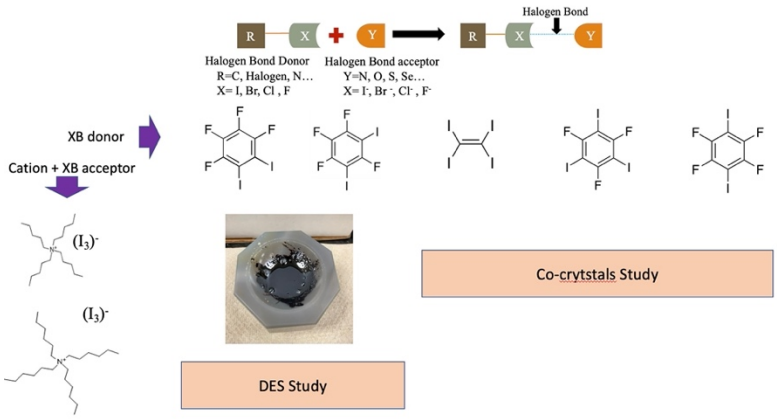
Ammonia sensing is crucial in various applications such as environmental gas analysis, automotive and chemical industries, agriculture, and the medical field. Detecting ammonia in ambient environments poses a challenge due to the interference caused by water vapor, as both water and ammonia molecules interact with sensing devices in similar ways. Given that water vapor concentrations often surpass those of ammonia, it is essential for ammonia sensing methods to exhibit high relative selectivity and be developed considering the interference of water. Despite the significance of this issue, many reported ammonia sensing methods in the literature, particularly those with environmental and biomedical implications, neglect the impact of water vapor, rendering their applicability in real-world scenarios questionable. Therefore, we present a novel sensing method capable of measuring ammonia vapor even in the presence of saturated water vapor. This method relies on the modulation of electrical conductivity in nanocomposite films (NCF) when exposed to both water and ammonia vapors. Our approach utilizes NCF composed of closely spaced silver nanoparticles separated by thin silica or polymer layers, serving as electrically conductive junctions sensitive to adsorbed ammonia molecules. The research focuses on the fabrication and optimization of these NCFs, elucidating the chemical mechanisms underlying their sensing properties. The results demonstrate excellent selectivity to moist ammonia vapor compared to water vapor alone. Importantly, the method exhibits high sensitivity and a low limit of detection in the sub-ppm range, even in the presence of interfering water vapor.

Poster #27

Exploring Cocrystals and Deep Eutectic Solvents based on halogen bonding for future advancements in drug development.

Madhushi Bandara, Hampton Warner, Victoria Critchley, Audrey Gasque, Arianna Ragusa, and Colin D. McMillen*, William T. Pennington*

Department of Chemistry, Clemson University.



Halogen bonding is a noncovalent intermolecular interaction that occurs between an electrophile and a nucleophile analogous to hydrogen bonding. This is often observed in compounds containing heavy halogens like iodine and bromine. When the halogen atom is covalently bonded to another atom or molecule, preferably to an electron-withdrawing moiety, an electrophilic region (sigma hole) is created on the halogen atom on the extension of the covalent bond while a nucleophilic region is created orthogonal to the covalent bond1. Type 2 halogen bonding in which the angle between the electrophile and nucleophile of neighboring molecules is 180° or almost linear, imparts directionality and tunability through the halogen bonding interactions. This can make extended networks such as chains, sheets, and 3D frameworks through self-assembly leading to many potential applications where structural design is important, such as in supramolecular chemistry, crystal engineering, and the pharmaceutical industry. The halogen bond donors are more hydrophobic compared to analogous hydrogen bond donors. Hence nearly all halogen bonded adducts are more lipophilic than analogous hydrogen bonded adducts. This feature of halogen bonding is used to enhance the drug permeability through cell membranes. In our studies, we use iodide and triiodide alkylammonium salts as halogen bond acceptors and iodofluorobenzenes as halogen bond donors to produce cocrystals via slow evaporation of the solvent at room temperature and pressure. The crystal structures are obtained using single-crystal diffraction and are useful to develop broader structural tendencies that can be applied to materials or pharmaceutical design. If the combination of halogen bond donors and acceptors does not produce a cocrystal, the potential implications are equally exciting. A liquid or eutectic reaction product can be characterized by thermal analysis techniques such as differential scanning calorimetry and thermal gravimetric analysis. Full mole

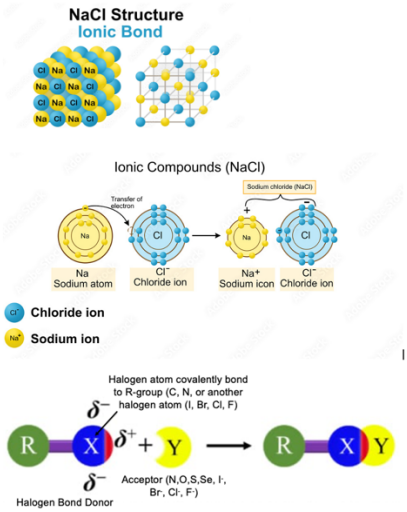
fraction studies plotted with predicted melting temperatures reveal any deep eutectic compositions in these halogen-bonded systems. Deep eutectic solvents (DES) are considered tunable solvents and a greener alternative to ionic liquids and conventional solvents due to their low vapor pressure and more benign constituents. DESs based on hydrogen bonding are well explored in literature while those based on halogen bonding is scarce. The very first DES based on halogen bonding was reported by Peloquin and coworkers in a mixture of 0.35-0.70mol% 1,3- dithiane and 0.65-0.30mol% 1,2-diiodo-3,4,5,6-tetrafluorobenzene with the eutectic point at 13.7°C4. DESs are involved in applications in metal deposition and synthesis, and an emerging area of DES study is in biotransformations which convert absorbed drugs into active agents or convert toxins into less harmful substances in the body. Traditionally biotransformation is performed in aqueous solvents since polar organic solvents denature enzymes. Hence, replacing polar solvents with DESs could allow the substrate to dissolve without denaturing the enzymes5. In the current study, a new class of DESs produced by triiodide alkylammonium salts and iodofluorobenzenes is introduced and characterized.

Authors acknowledge the financial support from NSF, Division of Chemistry, award CHE-2050042 (REU Program)

Poster #28

Investigating Cocrystal and Eutectic Formation in Specific Compositions: An In-depth Exploration

Maryelle Nyeck, Colin McMillen, and William Pennington
Department of Chemistry, Clemson University



Metal halides, compromising chemical compounds formed by the combination with one or more halogen atoms like fluorine, chlorine, bromine, iodide, or astatine, typically form negative ions (anions) when bonding with other elements. They play a crucial role in the formation of both eutectics and cocrystals. In eutectic systems, halides actively participate in the creation of mixtures with lower melting points by disrupting the crystal lattice and promoting components mixing. This phenomenon allows for the formation of eutectic mixtures, which consist of a ratio of two or more components that melts at temperatures lower than any of their individual constituents. Additionally, halides can be integral to the formation of cocrystals, crystalline materials composed of multiple molecular species held together by non-covalent interactions such as hydrogen bonds, π-π stacking, or halogen bonding. Within cocrystals, halides may serve as essential components, providing sites for halogen bonding interactions that contribute to the stability of the resulting crystalline structures. In both cases, the presence of halides can significantly influence the physical properties, stability, and behavior of the resulting eutectic mixtures or cocrystals. The specific interactions and properties depend on various factors, including the nature of the halide, its concentration, and its interactions with other components within the system. Organo-iodine, organic compounds characterized by atoms bonded to carbon atoms, often play a pivotal role in the formation of eutectics and cocrystals owing to iodine, unique properties and its versatility in various crystalline formations. These compounds actively participate in the creation of eutectic mixtures by engaging with both organic and inorganic compounds. Iodine is relatively large size and polarizability enable it to establish halogen bonds with other molecules, thereby lowering the melting point of the resulting eutectic mixture.

Moreover, organo-iodine contribute to eutectic formation by facilitating additional interaction like π-π stacking or hydrogen bonding, depending on the specific molecular arrangement. Frequently utilized in the formation of cocrystals, organo-iodine exhibit a remarkable ability to form robust halogen bond donors or acceptors, interacting with complementary functional groups in other molecules. These interactions play a crucial role in stabilizing the crystal lattice of the cocrystal and shaping its structural and physicochemical attributes. The presence of organo-iodine in cocrystals can enhance solubility, bioavailability, and other desirable characteristics, making them promise for pharmaceutical or material science applications. Overall, organo-iodine play a significant role in the formation of eutectics and cocrystals by contributing to intermolecular interactions that stabilize the resulting crystalline structures and modulate their properties.The current study aims to correlate intramolecular interactions with the structural motifs observed in compounds and to relate these interactions to physical quantum properties such as melting points, which are indicative of the formation of eutectics or cocrystal. Additionally, we seek to determine whether certain compositions lead to the formation of cocrystals and/or eutectics. Our study focuses on compositions involving choline halides and organo-iodine compounds. We aim to investigate the effects of mixing these components and explore questions such as the impact varying the proportions of each component, including metal halide salts. We aim to understand whether the presence of different ratios of these components still results in the formation of cocrystals and/or eutectics. Furthermore, we plan to introduce iodophenol as an organo-iodine compound and assess its effectiveness in forming cocrystals and/or eutectics in comparison to other compositions. The primary questions guiding our research include identifying the variable that can be manipulated, exploring different combinations of molecules, and investigating changes in stoichiometry.

Poster #29

A New Motif in Halogen Bonding: Cooperative S–Br···O, O···F, and F···F Interactions in the Crystal Packing of α, ω-Di(sulfonyl bromide) Perfluoroalkanes

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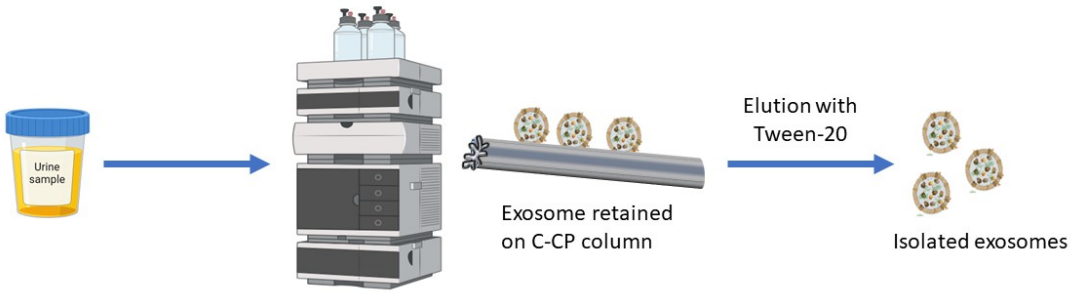
The first examples of S-Cl•••O halogen bonding complemented by short F•••F interactions between neighboring chains resulting in stabilized crystals of ClSO2(CF2)4SO2Cl and ClSO2(CF2)6SO2Cl were reported by us in 2018.1 Since then, other researchers suggested through Independent Gradient Model (IGM) studies of our crystallographic data that more noncovalent interactions between fluorine atoms on neighboring chains in addition to Cl•••Cl, Cl•••S, O•••F, and O•••S attractive associations can be found if one would look beyond the IUPAC's proposed 'less than the sum of the van der waals radii' criterion, insinuating that it should not be assumed to apply in every situation.2 With this, we are reporting samples of the related BrSO2(CF2)nSO2Br derivatives (n = 4, 6, 8, and others)3 which display stronger S-Br•••O halogen bonding interactions that are complemented slightly by O•••F as well as F•••F intermolecular interactions observed by X-Ray crystallography in addition to computational methods via IGM isosurface plots. Additional characterization (multinuclear NMR, FT-IR, and MS) of the disulfonyl bromide derivatives BrSO2(CF2)nSO2Br (n = 4, 6, 8) was also obtained in addition to preliminary spectroscopic evidence for BrSO2(CF2)2SO2Br and BrSO2CF2O(CF2)2OCF2SO2Br.

Poster #30

Isolation and Quantification of Human Urinary Exosomes Using a Tween-20 Elution Solvent from Polyester, Capillary-Channeled Polymer Fiber Columns

Md Khalid Bin Islam, and R. Kenneth Marcus
Department of Chemistry

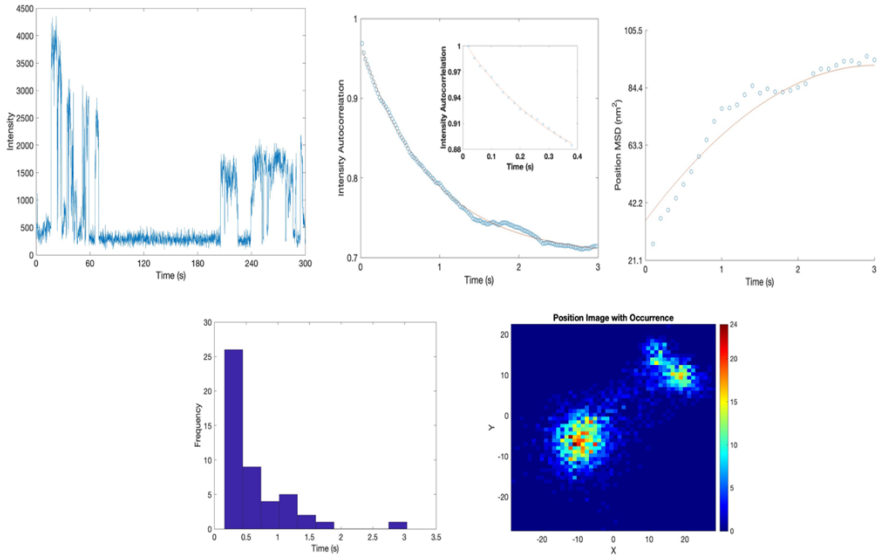


Extracellular vesicles (EVs), released by all cells, carry genetic materials that are crucial elements in several biological processes. Exosomes, a subset of EVs, range in size from 50 to 200 nm, are a type of membrane-secreted vesicle essential for intercellular communication. There is a great deal of interest in developing methods to isolate and quantify exosomes to study their role in intercellular processes and as potential therapeutic delivery systems. Most current EV isolation methods (i.e. ultracentrifugation, ultrafiltration etc.) suffer from practical challenges being time- and cost-intensive and result in EVs of low purity. Here, we present the optimization of Tween-20 to promote high throughput exosome elution from human urine on a cost-effective (~ $5/column) polyester capillary channeled polymer fiber column yielding excellent purities. A novel 10-minute two-step gradient method, employing 0.1% v/v Tween-20, efficiently isolated exosomes at a concentration of ~10^{11} EVs mL^{-1} from a 100 µL urine injection. Integration of absorbance and multi-angle light scattering detectors in standard HPLC instrumentation enables a comprehensive one-injection determination of eluted exosome concentration and sizes. Transmission Electron Microscopy confirms the structural integrity of the isolated vesicles, while the micro bicinchoninic acid (micro-BCA) protein quantification assay confirmed high-purity isolations ($5x10^{10}$ EVs μg^{-1} protein). The proposed method holds promise for a wide range of clinical and diagnostic applications, marking a significant advancement in C-CP based HIC research methodologies.

Poster #31

Charge carrier dynamics in single conjugated polymer chain

Ming Lei (a), and Jason McNeill (a)
Department of Chemistry



Conjugated polymers possess a high density of delocalized electrons and exhibit high absorption coefficients with electronic band gaps ranging from UV to near-infrared. However, the disordered or semicrystalline structure of the polymer leads to a complex energy landscape for charge carriers, characterized by trapping or dispersive transport. Therefore, a deeper understanding of the relationship between nanoscale structure and charge transport properties is vital for investigating and improving conjugated polymer-based device performance. In our lab, previous studies found that the fluorescence centroid displacement can be used to estimate the position of a single charge carrier in a conjugated polymer nanoparticle. The position can be recorded over time, showing the trajectory of the charge carrier. Furthermore, the fluorescence spectrum of the region within 1-3 nm of the polaron can be obtained, yielding a detailed map of the energy landscape. Previously, this charge carrier tracking technique was applied to conjugated polymer nanoparticles containing dozens or hundreds of polymer chains. In this work, technique will be modified and applied to single isolated conjugated polymer chain of PFBT (poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(1,4-benzo-{2,1,Ä≤,3}-thiadiazole) to obtain a more detailed chain segment level picture of charge transport and the energy landscape of conjugated polymers.

Poster #32

Toward an enantioselective preparation of diazacyclobutene (DCB) atropisomers and accessing rare heterocycles from vinyl sulfides DCBs

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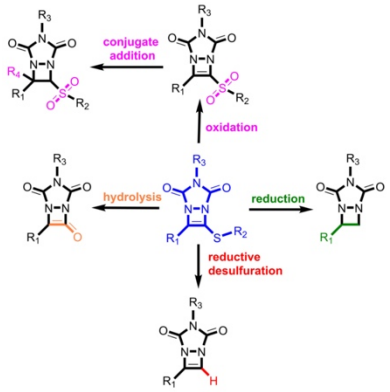


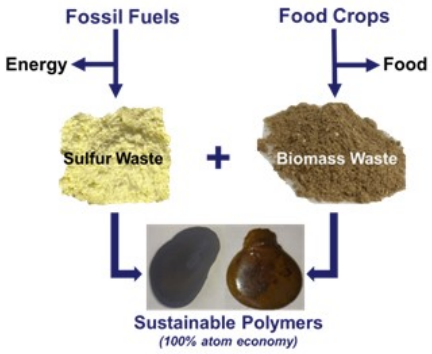
Nitrogen-containing heterocycles with different ring sizes are considered promising moieties in pharmaceutically active compounds. These nitrogen-containing compounds have significant applications in synthesis, particularly in pharmaceutical chemistry, chemical biology, and material science. Our group has recently developed a synthetic method leveraging the union of thioalkynes and triazolinediones to access diazacyclobutenes (DCBs) as a stable but rarely studied group of heterocycles. Remarkably, these diazacyclobutenes have exhibited potent antiparasitic activity against *Trypanosoma brucei*, the causative organism of african sleeping sickness. In our ongoing project, we are developing synthetic methods to expand on the molecular diversity of the DCB scaffold, aiming to enhance our understanding of its comprehensive antiparasitic capabilities. Notably, we have successfully oxidized the vinyl sulfide moiety of the DCB scaffold to the corresponding vinyl sulfone. This advancement propels our exploration towards the delivery of cuprate or other 1,4-nucleophiles, enabling the synthesis of alkylated, saturated diazetidines. Simultaneously, we are developing methodologies for the hydrolysis of the vinylsulfides moiety of the DCB under protic or Lewis acid conditions. This endeavor is poised to provide access to the relatively rare aza-beta-lactam scaffold, a transformation of both synthetic and biological significance, given the prevalence of beta-lactam functionality in many potent drug molecules, such as Penicillins. Furthermore, our investigation extends to the conformational fluxionality of bicyclic DCBs. Our findings reveal that the scaffold undergoes rapid conformational interconversion at room temperature through double nitrogen inversion (ΔG = 13.4 ± 0.7 kcal/mol). Building upon this knowledge, we are actively engaged in the development of an enantioselective synthesis of DCB

atropisomers. This involves screening various H-bond and Bronsted acid chiral catalysts to facilitate the reaction. Our current innovative techniques aim not only to expand the molecular complexity and diversity of DCBs but also to deepen our exploration of their holistic antiparasitic activity against the *Trypanosoma brucei* parasite. Through these endeavors, we hope to contribute to the advancement of both synthetic methodologies and our understanding of the biological potential of these intriguing nitrogen-containing heterocycles.

Poster #33

Diverse Reactivity of Lignin Model Compounds with Elemental Sulfur: Mechanistic Insights and Sustainable Polymer Development

Nawoda L. Kapuge Dona, and Rhett C. Smith
Department of Chemistry



This century has seen rapid growth in efforts to utilize plant-based materials to replace petroleum-based precursors towards minimizing environmental impact. Lignin is the most underutilized component of biomass waste and the primary aromatic biopolymer found in high abundance, and will play a key role in replacing petrochemical aromatics. Given the molecular complexity and low solubility of lignin, the study of model compounds holds promise for understanding reactivity patterns in lignin and thus advancing lignin valorization. Sulfur is another vastly underutilized waste product, derived from fossil fuel refining processes. Surprisingly, the fundamental reactivity of lignin model compounds with elemental sulfur is largely unknown. In this work, nine lignin model compounds were reacted with elemental sulfur to elucidate the S,ÄìC bond-forming reactions these model compounds undergo. Each of the nine model compounds was reacted with elemental sulfur in three sulfur: organic reactant ratios (2:1, 4:1 and 9:1) and at two temperatures (180 oC or 230 oC). Product mixtures were characterized using 1H NMR spectrometry and GC-MS analysis. Several distinct mechanisms were observed for the reactivity between lignin models and elemental sulfur, including inverse vulcanization, S,ÄìC(allylic/benzylic) bond formation, S,ÄìC(aryl) bond formation, intramolecular cyclization, self-condensation, C,ÄìC Sigma-bond scission, and C,ÄìO Sigma-bond scission steps. Building on these initial studies, the evaluation of thermo-morphological and mechanical properties of polymers made from lignin model compounds and sulfur was undertaken to gain insight into potential applications and structure-property relationships. Polymers were initially characterized by elemental analysis, Fourier-transform infrared spectroscopy, and scanning electron microscopy with energy dispersive X-ray analysis (SEM/EDX). Thermal properties were assessed by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The compressive, flexural, and tensile strength of materials were also analyzed and found to be competitive with traditional mineral building products.

Poster #34

Saturation-Transfer Difference NMR Studies on the Influence of Salt on Binding between Nanoplastic and Amino Acids

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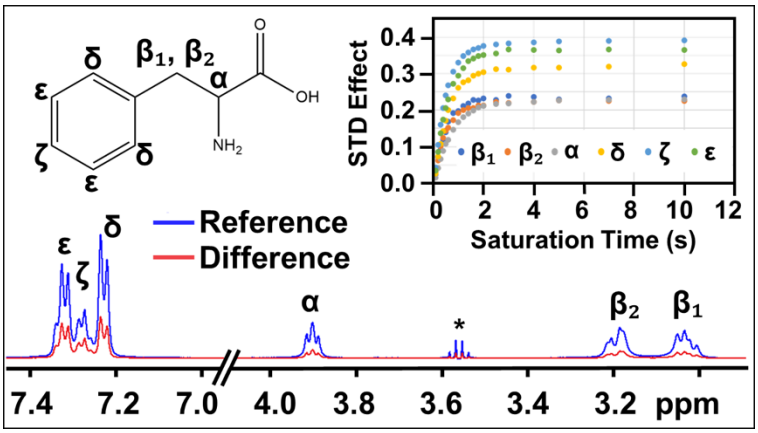
(a) Department of Chemistry, Clemson University



Nuclear Magnetic Resonance (NMR) spectroscopy is a versatile analytical technique for studying the structure and dynamics of molecules. Solution-state NMR covers a range of techniques that offer important insights into the structure and behavior of molecules in solution. One method for investigating molecules bound to nanoparticles is the Saturation-Transfer Difference (STD) experiment. This approach yields important insights into both the binding epitope and the affinity of the ligand toward the receptor. In STD NMR, specific irradiation of the protons in the receptor results in transferring saturation to the ligands via intermolecular dipolar coupling. The difference in NMR signal strength between experiments in which the receptor resonances are saturated or unsaturated discloses which protons of the small molecule are situated close to the surface of the receptor. We studied the ability of several plastic nanoparticles to bind different amino acids and their modes of interaction, and investigated how salt influences the binding. These results can aid in developing a better understanding of the fate and impacts of plastic nanoparticles in natural waterways and their possible health impacts.

Poster #35

Investigating the structure-activity relationship of Oxadiazon derivatives against the Toxoplasma gondii infections in human

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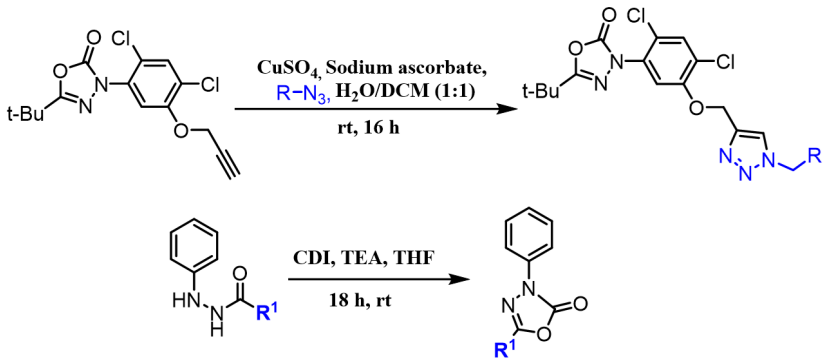
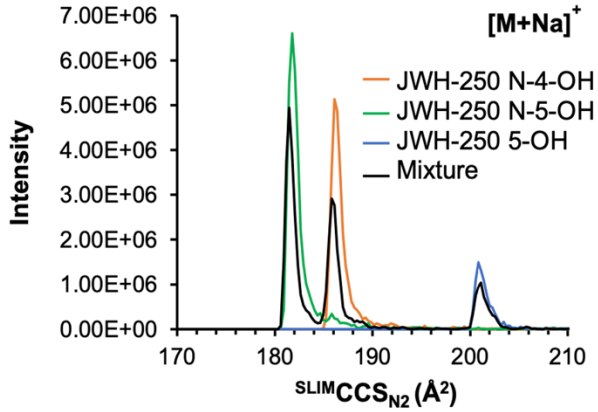


Toxoplasmosis, a parasitic infectious disease caused by Toxoplasma gondii which belongs to the Apicomplexa phylum, has adverse effects like brain, eyes, and other organ damage on the vast majority of the human population. Drugs currently being used to treat toxoplasmosis are not fully compatible with the diseases having severe side effects. Our previous protoporphyrinogen oxidase (PPO) enzyme study showed that a type of herbicidal synthetic compound belonging to oxadiazon groups is capable of inhibiting plant T. gondii that generally propagates through heme and chlorophyll biosynthetic pathway. Using the oxadiargyl and oxadiazon compounds as the potential lead, we synthesized a new library of 38 compounds by structural modification. Some compounds showed better inhibition activity against T. gondii PPO with IC50 values less than 2.5 ŒºM. Further structural analysis will lead us to synthesize more active compounds and eventually help to develop more compounds with improved inhibition activity against T. gondii infections.

Poster #36

Separation of New Psychoactive Substances and Xylazine Metabolite Isomers using SLIM High-Resolution Ion Mobility-Mass Spectrometry (HRIM-MS)

Ralph Aderorho1, Shadrack Wilson Lucas2, and Christopher Donald Chouinard
Department of Chemistry



New psychoactive substances (NPS) such as synthetic cannabinoids (SC) are often laced with xylazine, a common and potent veterinary sedative. This adulteration increases potency thereby altering brain chemistry, causing hallucinations, euphoria, and potentially death. NPS and xylazine undergo metabolic transformations yielding complex and active metabolic isomeric mixtures. Traditional analytical methods face challenges in resolving these isomers, hindering accurate pharmacokinetic studies, and therefore it is critical to develop techniques for accurate identification. This study leverages Structures for Lossless Ion Manipulations (SLIM), a high-resolution ion mobility (HRIM) technique that enables improved separation of metabolite isomers. This innovative approach holds promise for advancing pharmacological studies, facilitating the identification and quantification of NPS and xylazine metabolites, and enhancing the understanding of their metabolic pathways.

Sample mixtures were prepared (1 µg/mL) and then derivatized using dansyl chloride to target hydroxyl and amine groups in different positions. The mixtures were analyzed by direct injection using an Agilent 1290 Infinity II UHPLC coupled to MOBILion Systems MOBIE HRIM SLIM and Agilent 6546 QTOF. The SLIM has a 13 m pathlength IM region containing nitrogen or helium buffer gas maintained at ~25 °C and 2.5 Torr. SLIM TW frequency/amplitude were optimized for isomer separations and sensitivity. Additionally, all samples were analyzed using an Agilent 6560 IM-QTOF, specifically for acquiring accurate reference CCS values. All data were subjected to PNNL Pre-Processor frame compression, and analysis was performed with Agilent MassHunter IM-MS Browser 10.0.

The collision cross sections (CCS) of all NPS compounds were measured in the range of 154.4 to 206.3 Å² for both protonated [M+H]+ and sodiated [M+Na]+ ions. Notably, a baseline separation was achieved for isomeric synthetic cannabinoid (SC) metabolites, including JWH-250 5-hydroxyindole (203.7 ± 0.1 Å²), JWH 250 N-(4-hydroxypentyl) (184.3 ± 0.1 Å²), and JWH 250 N-(5-hydroxypentyl) (183.8 ± 0.1 Å²), all observed as sodiated species at m/z 374.173. However, only partial separation was observed for JWH-018 4-hydroxyindole (206.4 ± 0.1 Å²), JWH-018 N-(5-hydroxypentyl) (193.9 ± 0.1 Å²), and JWH-018 6-hydroxyindole (206.3 ± 0.1 Å²) as sodiated species at m/z 380.163. In contrast, complete overlap was observed for 3-hydroxy xylazine (154.4 ± 0.1 Å²) and 4-hydroxy xylazine (154.4 ± 0.1 Å²), both as protonated species at m/z 237.105. These isomers differ only in the position of a hydroxyl group.

In an effort to improve IM separation, a derivatization reaction using dansyl chloride was employed to selectively target phenolic alcohols present in several of the metabolites. This led to a major product ion at m/z 591.233 for the JWH-018 metabolites and mono- and di-sulphonate esters with m/z 470.156 and 703.207, respectively, for the xylazine metabolites. Baseline separation of isomers with a peak-to-peak resolution of Rpp > 1.5 was achieved for both isomeric groups. However, the formation of a di-sulphonate ester with m/z 703.207, resulting from the reaction of xylazine metabolites with dansyl chloride, introduced plane chirality, leading to the formation of atropisomers exhibiting a unique structural characteristic.

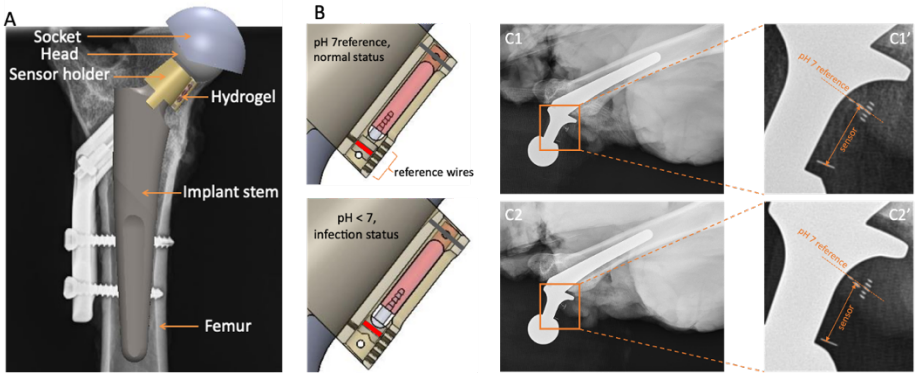
The novel aspect of this research shows the first demonstration of SLIM-based separation of synthetic cannabinoids and xylazine metabolites using dansyl chloride derivatization.

Poster #37

Detection of Hip Implant Infection with an implantable Sensor via plain radiography

Rong Wang (a), Sachindra D. Kiridena (a), Uthpala N. Wijayaratna (a), Kendra Boyd (b), Halli Wall (b), Katherine Traver (b), Joshua Finkel (c), Thomas P. Schaer (d), Rachel Butler (d), Phillip C. Moschella (e), John D. Adams (f), John D. DesJardins (c, g), and Jeffrey N. Anker (a, c, g)

(a) Department of Chemistry, (b) Chemistry/Bioengineering Undergraduate Creative Inquiry Program, (c) Aravis BioTech LLC., Greenville, SC, (d) School of Veterinary Medicine, University of Pennsylvania, Philadephia, PA, (e) Department of Emergency Medicine Prisma Health-Upstate, Greenville, SC, (f) Department of Orthopedic Surgery Prisma Health-Upstate, Greenville, SC (g) Department of Bioengineering



Hip replacement surgeries improve patient mobility and quality of life, however, infection is still a devastating complication in about 0.5-2% of cases. Sensors are needed to detect infection early to avoid the need for revision surgery and to monitor infection during antibiotic treatment to ensure eradication after either irrigation & debridement or replacement with temporary antibiotic-impregnated spacers. Synovial infection markers, such as glucose, pH, lactate concentrations, C-reactive protein, alpha defensin, etc. may be helpful in defecting early infections. Studies show that synovial joint fluid pH decreases from pH 7.5 to around 6.7 during infection. However, joint aspiration is required to carry out synovial fluid for infection analysis, which is painful and needs to be performed by a radiologist. A synovial fluid pH sensor based on a pH-responsive poly (acrylic acid) hydrogel was developed, which can be attached to prosthetic hips. The sensor would enable non-invasive early detection and monitoring of hip infections using plain radiography, which is already routinely acquired during patient follow-up visits.

The pH-responsive poly (acrylic acid-co-octyl acrylate) hydrogel was prepared by UV light-initiated free radical polymerization of acrylic acid and n-octyl acrylate. The hydrogel contracts at low pH, moving a radio-dense tantalum bead relative to a fixed pH 7.0 reference marker as evident in the radiograph. The calibration curve shows a sigmoidal tantalum bead position vs. pH, with a dynamic range of pH 4-7 and pK_aof 5.23. The sensor responds well in the physiological pH 6.5 and 7.5 range, with excellent reversibility and a 30-minute response time. The inter-observer reliability shows that measured pH values fit well with the actual pH values, the average inter-

observer precision is 0.03 pH unit, and the accuracy is 0.08 pH unit. A similar sensor worked in a live rat peritoneal dialysis model. To further measure in vivo infection-relevant acidosis of synovial fluid, the sensor design was miniaturized for subsequent sheep study and optimized for more reproducible manufacture and integration into a canine hip prosthesis. The improved hydrogel sensor has a 3D-printed biocompatible sensor holder and extra screws to fix the hydrogel position and prevent potential displacement over time. While autoclaving the sensor once did shift the calibration, subsequent autoclaving steps showed no further effects.

Preliminary sheep carcass study results show the feasibility of measuring local pH in synovial fluid at hip implants, and the sensor enables non-invasive early detection and monitoring of hip infection using plain radiography. In vivo sheep studies are planned in the near future.

Poster #38

Interfacial Diffusion in Associative Polymers: MD Simulation Study

Rosita Sivaraj (a), Gary Grest (c), and Dvora Perahia (a) (b)
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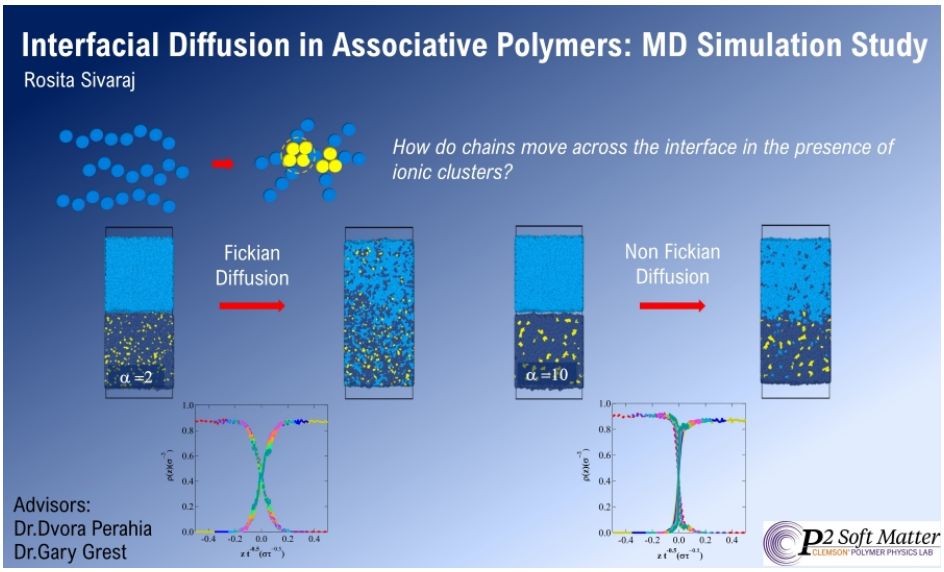
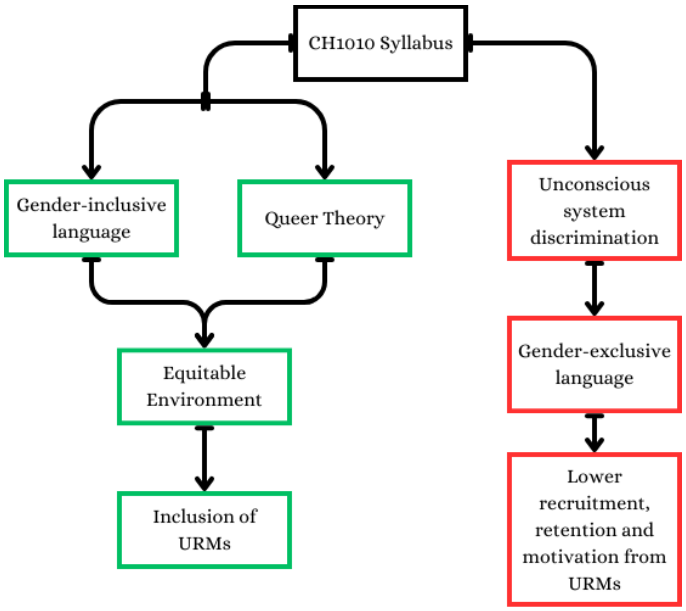


Polymer dynamic behavior at interfaces often defines the stability and control function of macromolecules in a broad range of applications. The interfacial behavior polymers that consist of highly interacting groups, such as ionizable segments, differ significantly from that of van-der Waals polymers, where tethering a few associating groups to a polymer backbone significantly affects the polymer mobility due to the formation of ionic clusters. Using molecular dynamics (MD) simulations, this study explores the interfacial dynamics at the associative/non-associative polymers interface using a bead-spring model starting with a length of 20 beads per chain with interacting beads of varying interactions 1 to 10 kBT typical to the van der Waals interactions and hydrogen bonds. We find that the interfacial structure of the interacting polymers changes as the interaction strength of the associating groups is varied and affects the interdiffusion across the interface. With increasing interaction strength, clusters grow in bulk, acting as physical crosslinkers, diminishing chain mobility in bulk and across the interfaces. The diffusion across the structured interface and degree of interpenetration as a function of interaction strength, chain length and polymer topology will be discussed.

Poster #39

Queering the CH 1010 General Chemistry Syllabus

Ruben Sousa (a), and Matthew Voigt (a)
(a) Department of Engineering and Science Education

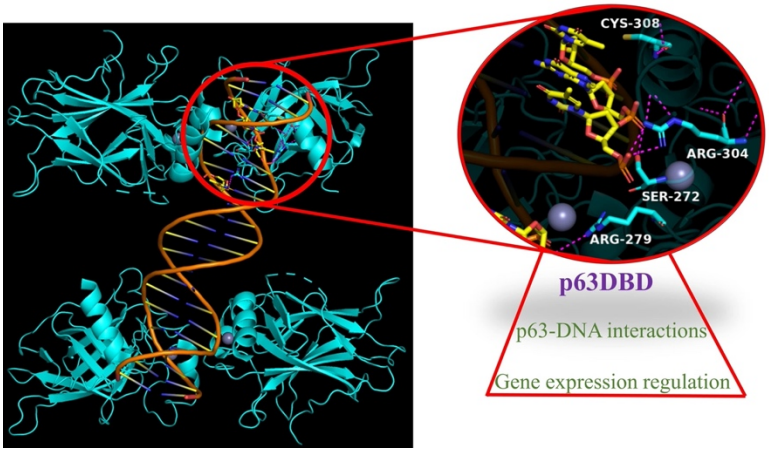


In this work, we present a theoretically-driven revamped syllabus for CH1010 General Chemistry at Clemson University. Different components were added and changed, such as inclusive wording, community expectations and instructor introductions, and the rationale and description for the changes is also included. Resources such as textbooks and syllabi are generally not written in inclusive language, in big part due to unconscious systemic bias in language and disciplinary norms. These resources are usually the first interaction a student has to a particular field, and it makes a difference whether they,Äôre approached with gender-inclusive vs gender-exclusive language. Including something as simple as pronouns in your introduction can be the difference between having a student showing up for their first class excited rather than scared, which can be the key factor for retention of underrepresented and sexually-marginalized students in STEM. Teaching a first-year General Chemistry class in a research-intensive school means that instructors are likely to share the same coordinated syllabus, and there might not be a lot of leverage for changes. By aligning Queer Theory and syllabi design, we allow General Chemistry to challenge systemic issues of inequity and connect each student to the class, regardless of their social identities, while simultaneously improving the classroom environment for every student. Future work will involve getting resources like the Office for Teaching Effectiveness and Innovation, the Department of Undergraduate Studies and the Division of Inclusion and Equity included in the conversation when developing syllabi and setting the tone for inclusivity in first-year classes at Clemson.

Poster #40

Understanding the Structural Consequences of P63DBD Mutations Through Comparative Computational Approach

Salini Dimanthika Yapa (a), Samuel Kwain (a), Daniel C. Whitehead (a), and Brian Dominy (a)
(a) Department of Chemistry

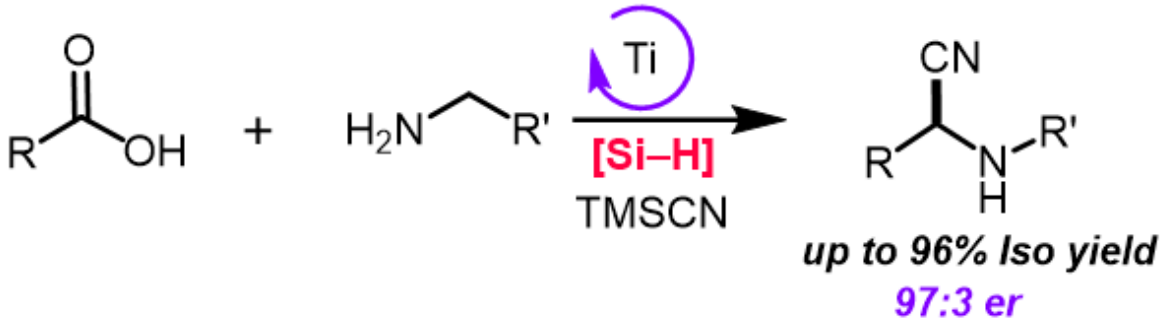


p63, a member of the p53 family of transcription factors, plays vital roles in various cellular processes such as epithelial cell development, cell cycle regulation, apoptosis, and tumorigenesis. The p63 DNA binding domain (p63DBD) is pivotal for its interaction with specific DNA sequences and subsequent gene expression regulation. Point mutations occurring in this domain can significantly impact the protein's functionality. In this computational study, we investigated the structural implications of several p63DBD mutations (S272N, R279C/H/Q, R304P/Q/W, C308Y H208Y, C269Y, and C273Y) identified in patients with conditions such as ectodermal dysplasia, split hand/foot malformation, and orofacial clefts. We developed a model of the wild-type (WT) and mutant forms of the protein using molecular modeling and molecular dynamics simulation techniques. The analysis conducted through molecular dynamics (MD) and molecular mechanics/Poisson‚ÄìBoltzmann surface area (MM-PBSA) calculations suggest that these mutations in p63DBD may exhibit dual effects - directly impacting DNA binding and inducing instability in the protein structure. Both of these consequences could contribute to developing genetic syndromes involving malformations and potentially influence other cellular processes regulated by p63. Understanding the structural and functional implications of these mutations is crucial for unraveling the molecular mechanisms underlying these syndromes and for the development of potential therapeutic interventions

Poster #41

Titanium Catalyzed Multi-functionalization of Carboxylic acids for The Synthesis of Chiral Amines

Samirah Muhammad (1), Giovani Gutierrez (1), Jason A. Wilt (1), and Dr. Byoungmoo Kim (1)
(1) Department of Chemistry



Chiral amines are important motifs that are present in many bioactive molecules, natural products, and pharmaceuticals. Therefore, there has been a continuous demand for more efficient enantioselective methods to synthesize chiral amines. The Strecker reaction is one of the well-established ways for the enantioselective synthesis of chiral amines, which involves carbonyl, an amine, and cyanide starting materials. However, the carbonyl starting materials are often unstable which limits the utility of this reaction. On the other hand, the corresponding carboxylic acids are desirable candidates to use since they are bench stable, non-toxic, inexpensive, and abundant building blocks. Despite these advantages, there are only a few examples of the reductive Strecker reaction using carboxylic acids and there are no known enantioselective variants. Additionally, current examples of the reductive Strecker reaction often use precious metal catalysts such as iridium, which can be expensive and impact scalability. To address these challenges, we describe our efforts in the Kim Group employing a first-row transition metal, specifically titanium, as a catalyst, which is inexpensive, non-toxic and offers diverse reactivities. Our method uses a single titanium catalyst to take various carboxylic acids to enantio-enriched amine products in one-pot without the need for multiple catalysts or intermediate purification making this method more efficient. Our current focus is to demonstrate a gram scale synthesis of the method and expand the multi-catalytic strategy to the catalytic decomposition of plastic wastes.

Poster #42

Accessing Rare Heterocycles from Electron-rich Alkynes and Nitrogenous Electrophiles

Samuel Kwain (a), Brock A. Miller (b), Chandima J. Narangoda (c), Ugochukwu C. Ibeji (a), Aysiah Gibbs (a), James Aboko (a), Brian N. Dominy (a), and Daniel C. Whitehead (a)

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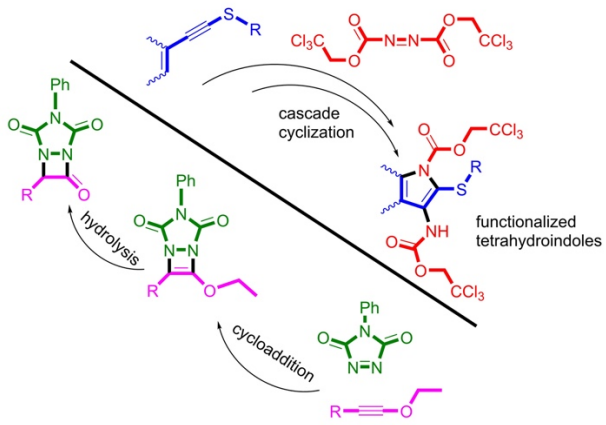
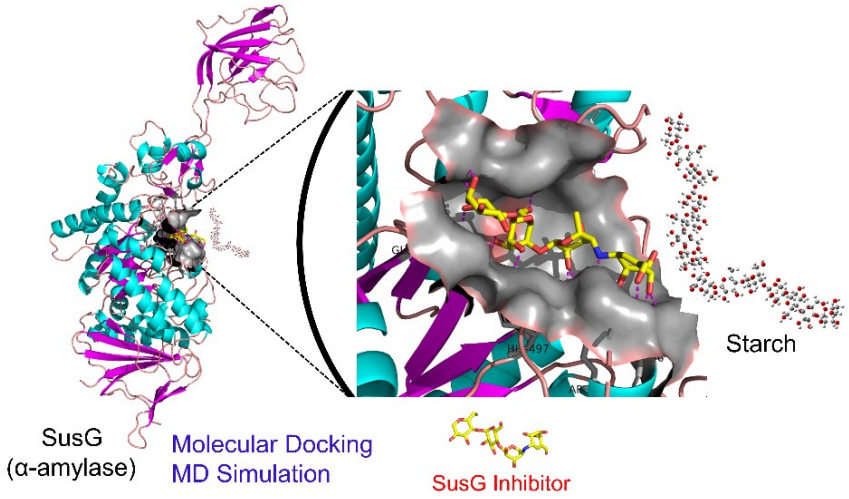


Nitrogen-containing heterocyclic compounds have shown significant utility in synthesis, particularly in pharmaceutical chemistry, chemical biology, and materials science. Despite the advancement in this area, methods targeting the synthesis of densely substituted diazahetrocycles, specifically 3-1,2-diazetine (diazacyclobutene) are significantly limited and remain the subject of active research. In recent times, our group has successfully developed an efficient strategy to access the infrequent densely substituted diazacyclobutene motif. This approach involves a formal [2 + 2] cycloaddition between electron-rich alkynes (thioalkynes and ynamides) and nitrogenous electrophiles such as azodicarboxylates and triazolinediones. This innovation not only provides easy access to the motif but also highlights the notable antiparasitic activity exhibited by the resulting diazacyclobutenes against Trypanosoma brucei ,Äì the causative organism of human sleeping sickness. In our current study, we have developed an improved method to access rare electron-rich alkynyl ethers, and subsequently, harnessed their reactivity with nitrogenous electrophiles through Lewis acid-catalyzed cyclization to access the diazacyclobutene motif. Detailed DFT calculations were employed to understand the differences in chemical reactivity between the electron-rich alkynes (thioalkynes, ynamides, and alkynyl ether) and the nitrogenous electrophiles in accessing the motif. Additionally, we have also developed a unique strategy that proceeds through a cascade reaction between ene-yne sulfides and azodicarboxylate, leading to the formation of alpha-iminothioimidate bearing an alpha-beta unsaturated imine. This intermediate readily undergoes intramolecular 1,4-cyclization, resulting in the formation of highly functionalized tetrahydroindoles.

Poster #43

Molecular Modelling-Aided Discovery of Small Molecules for the Selective Inhibition of the Polysaccharide Metabolism in Human Gut Microbes

Samuel Kwain (a), Kristi J. Whitehead (b), Brian Dominy (a)*, and Daniel C. Whitehead (a)*, and Daniel C. Whitehead (a)
(a) Department of Chemistry and (b) Department of Biological Sciences



The human gastrointestinal (GI) microbiota is the residence of millions of microbes that profoundly influence the host development and health. Among the resident microbes in the gut ecosystem, Bacteroidetes is the dominant phylum, with Bacteroides as the well-studied genus. Bacteroides spp. including B. fragilis (Bf) and B. thetaiotaomicron (Bt) exacerbate several chronic gut-associated diseases including ulcerative colitis, inflammatory bowel disease, celiac disease, and colorectal cancer. In addition, several studies have also found an increase in the population of some Bacteroides spp. in patients genetically at-risk for Type I diabetes mellitus (T1D) and in patients exhibiting clinical T1D. Interestingly the members of the Bacteroides genus possess a unique Starch Utilization System (Sus) used to metabolize complex starch molecules in the human GI microbiota as their main source of energy. Our lab previously reported that inhibition of the Sus of the members of the Bacteroides genus offers a potential druggable target to develop an effective therapy to selectively moderate the growth of these organisms in the human GI microbiota. In the present study, we targeted SusG, an Œ±-amylase, which is a principal component of the Bt Sus as a module receptor in a structure-based drug design to uncover small molecules (SK1-SK8) with potent selective inhibition against members of the Bacteroides genus. This was achieved through molecular modelling strategy using density functional theory (DFT), molecular docking, and molecular dynamics (MD) simulation to design the small molecule competitive inhibitors against the SusG protein. To confirm the inhibitory potency of the compounds we performed in vitro bioassay studies of the compounds against Bt

cultured in minimal media containing glucose, potato starch or pullulan as the main carbon source. The results revealed that the compounds are non-microbicidal and selectively inhibit the Bt Sus. The preliminary results from this work suggest that our molecular modelling strategy could be used to develop an effective therapy to selectively moderate the members of the Bacteroides genus in the human GI microbiota. This presentation will describe the molecular modelling strategy, synthesis and biological evaluation of SK1,àíSK8 as potential inhibitors of Bt Sus.

Poster #44

Structure and Dynamics in Polyelectrolyte Aqueous Solutions in Non-linear Shear Flows: A Molecular Dynamics Simulation Study

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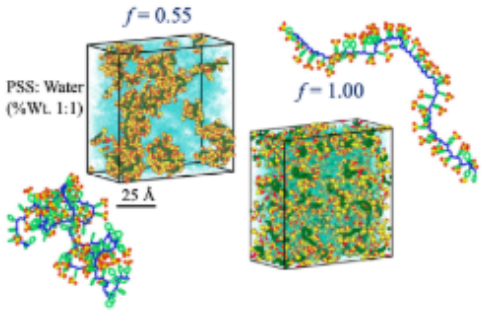

The interactions of polyelectrolytes with water are multifaceted, where this highly polar solvent preferentially resides in the vicinity of the ionic domains and concurrently collapses the hydrophobic polymer backbone, forming inhomogeneous dynamic systems. Their response to shear is at the core of their function and is of particular significance to novel recycling and upcycling strategies for waterborne plastic waste. A molecular-level insight into distinct dynamics of ionic assemblies and hydrophobic domains of polyelectrolytes in water is attained by fully atomistic molecular dynamics simulations using a model ionizable polymer, sulfonated polystyrene, PSS (molecular weight ~ 15 kg/mol), 37 chains at sulfonation fractions f= 0.55 and 1.00, neutralized with Na+ counter ions in Tip4p-fb water model. The systems phase segregates at f= 0.55, and increasing f forms co-continuous hydrophilic and hydrophobic domains. As a function of increasing shear time, the system displays an initial elastic response followed by shear rate-dependent and ionic fraction-dependent stress overshoot and, eventually, a steady state. At high shear rates, ionic assemblies break and rearrange, and coiled polymer chains fully open up. Chain orientation effects dominate the shear response of polyelectrolyte aqueous solutions.

Poster #45

Electrically Conductive Metal-Organic Frameworks

Shiyu Zhang (a), Ashok Yadav (a), Paola A. Benavides (a), Wei Zhou (b), and Sourav Saha (a)

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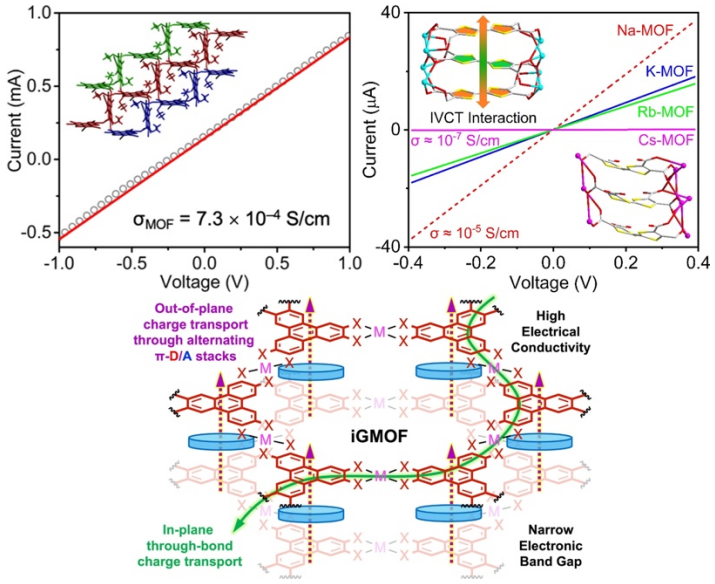

Electrically conductive Metal-organic frameworks (MOFs) have become one of the most promising electronic materials due to their diverse potential applications in supercapacitors, chemiresistive sensing, electrocatalysis, light-harvesting systems, etc. However, constructing highly electrically conductive MOFs requires a profound understanding of their structure-property relationships. Electrical conductivity is a product of two parameters: charge carrier concentration and charge mobility. While redox-active ligands, metal ions, and/or guest molecules supply charge carriers, charge mobility depends on the efficacy of charge transport pathways, which can be classified into the following categories: (1) through-bond: via metal-ligand covalent coordination bonds and conjugated π-bonds; (2) through-space: π-stacked ligands and redox hopping; (3) guest molecules-promoted pathway. Herein, we present three recent works based on through-bond charge transport pathway strategy, through-space charge transport pathway strategy, and dual through-bond and through-space charge transport pathway strategy. Firstly, we have constructed a new intrinsically conducting 3D framework [Ag2(HATHCN)(CF3SO3)2]n by employing a highly π-acidic HATHCN ligand, which assumed a paramagnetic HATHCN•− radical anion character by acquiring electron density from the TfO− anions involved in the anion-π interaction and facilitated charge movement along the staircase-like [-Ag+-HATHCN-]∞ chains. As a result, the MOF displayed a narrow band gap (1.35 eV) and promising electrical conductivity (7.3 × 10−4 S/cm). Through-space pathway strategy: we have constructed four novel alkali-metal-based (Na, K, Rb, and Cs) 3D-MOFs with continuous π-stacks using an electron-rich TTFTC ligand. Due to the different extent of π-π interactions and aerobically

oxidized TTFTC•+ population, these MOFs enjoyed varying degrees of TTFTC/TTFTC•+ intervalence charge transfer (IVCT) interactions, which commensurately affected their electronic and optical band gaps and electrical conductivity. Having the shortest dπ–π (3.39 Å) and the largest initial TTFTC•+ population (~23%), the oxidized Na-MOF 1-ox displayed the narrowest band gap (1.33 eV) and the highest room temperature electrical conductivity (3.6 x 10–5 S/cm), whereas owing to its longest dπ–π (3.68 Å) and a negligible TTFTC•+ population, neutral Cs-MOF 4 exhibited the widest band gap (2.15 eV) and the lowest electrical conductivity (1.8 x 10–7 S/cm). The freshly prepared but not optimally oxidized K-MOF 2 and Rb-MOF 3 initially displayed intermediate band gaps and conductivity, however, upon prolonged aerobic oxidation, which raised the TTFTC•+ population to saturation levels (~25 and 10 %, respectively), the resulting 2-ox and 3-ox displayed much narrower band gaps (~1.35 eV) and higher electrical conductivity (6.6 x 10-5 and 4.7 x 10–5 S/cm, respectively). Dual through-bond and through-space charge transport pathways strategy: we have constructed via an elegant bottom-up method the first π-intercalated GMOF (iGMOF1) featuring built-in alternate π-donor/acceptor (π-D/A) stacks of CuII-coordinated electron-rich HATP ligands and non-coordinatively intercalated π-acidic HCTP molecules, which facilitated out-of-plane charge transport while the hexagonal Cu3(HATP)2 scaffold maintained in-plane conduction. As a result, iGMOF1 attained a higher bulk electrical conductivity and much smaller activation energy than Cu3(HATP)2 (σ=25 vs. 2 S/m, Ea=36 vs. 65 meV), demonstrating that simultaneous in-plane (through-bond) and out-of-plane (through πD/A stacks) charge transport can generate higher electrical conductivity in novel iGMOFs.

Poster #46

Electric Field Gradient at Nanostructured Insulating Electrode Surface

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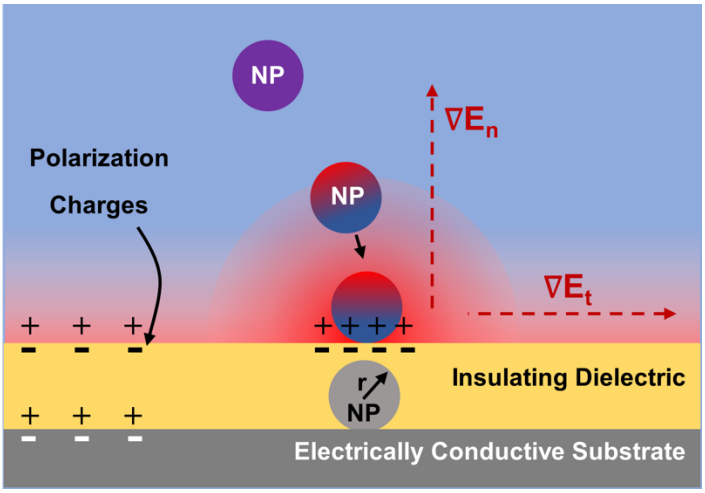
Department of Chemistry, Clemson University

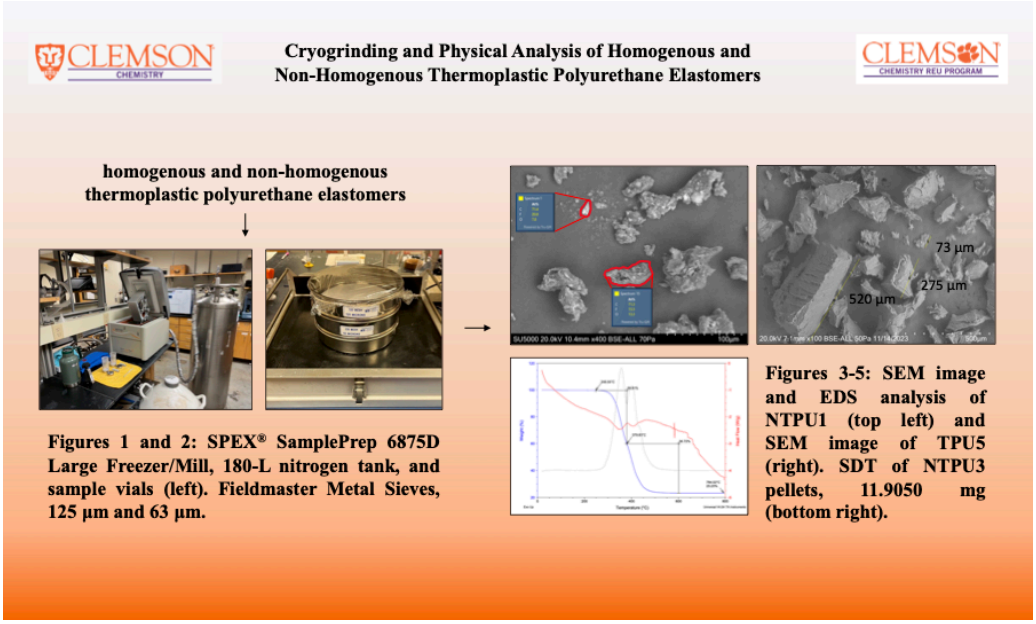


Nanostructured dielectric electrodes (NSDE) have been fabricated capable of producing a nonuniform electric field. The field gradient was characterized and the field intensity was estimated using electrostatic force microscopy (EFM). NSDE will be used to direct the dielectrophoretic assembly of nanoparticles into nanoclusters at the NSDE surface in future experiments.

Poster #47

Cryogrinding and Physical Analysis of Homogenous and Non-Homogenous Thermoplastic Polyurethane Elastomers

Timothy Whitesell (a), Marcia Reeves (a), David Helm (a), and Joseph Thrasher (a)
(a) Department of Chemistry



Commercially available polycaprolactone-based thermoplastic polyurethane (TPU) elastomer and non-homogenous elastomer products were chosen for cryogrinding and analysis. For this presentation, each product variant is generically named, the TPUs referred to individually as “TPU1,” “TPU2,” etc. The three non-homogenous TPUs being “NTPU1,” “NTPU2,” and “NTPU3.” The original form of all variants are in the form of colorless elliptical, cylindrical, or miscellaneous shaped pellets of average 4.8 mm in length and 3.2 mm in width. The goals include obtaining a product to a maximum size of <63 µm (longest diameter) with narrow distribution through cryogrinding, minimal molecular weight (MW) reduction, minimal metal contamination, and acquiring data on potential thermal and compositional properties changes due to the process of grinding. With this, we are reporting the methods and results of cryogrinding, particle size analysis via scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDS), thermal gravimetric analysis (TGA), and differential scanning calorimetry (DSC). Our industrial sponsor obtained results for particle size distribution via MasterSizer (light scattering), MW distribution via gel permeation chromatography (GPC) and trace metal analysis via inductively coupled plasma mass spectrometry (ICP-MS).

Poster #48

Oxygen sensing in 3D printed bone scaffolds via X-ray excited luminescent chemical imaging

Vigjna Abbaraju (a), Karim Ameziane (b), Hannu V√§lim√§ki (b), Sriparna Bhattacharya (c), Jonathan Massera (b), Pasi Kallio (b), and Jeffrey N. Anker (a), (d)

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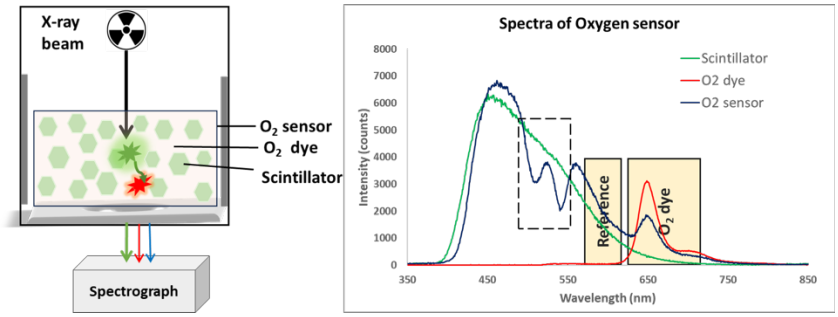
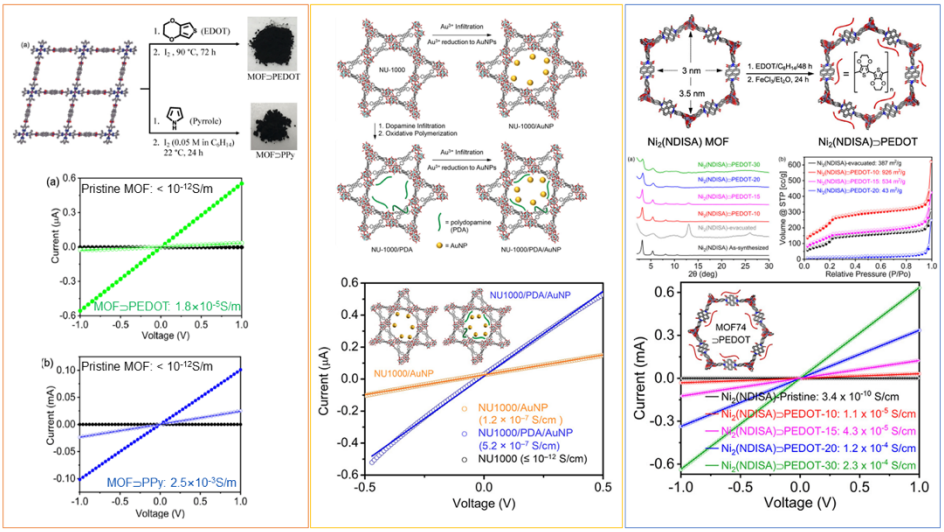


Understanding how cell growth in the bone scaffolds impact oxygen concentrations is essential for developing effective bone replacement scaffolds. X-ray radiography provides high-contrast images in deep tissues but lacks chemical sensitivity while fluorescence oxygen sensing is limited by light scattering in tissue. Nonetheless, X-ray excited luminescent chemical imaging (XELCI) enables biochemical sensing such as pH with local specificity and submillimeter resolution through tissue. Therefore, we developed an X-ray luminescent oxygen sensor to integrate it to a 3D printed bone scaffold for monitoring oxygen concentrations using our XELCI scanner. Previously, our collaborators from Finland demonstrated imaging changes in oxygen concentration within the bone scaffold during the oxygen perfusion using an oxygen sensitive dye with LED excitation. In our work, we fabricated sensor film consisting of both a scintillator to generate light locally and an oxygen sensitive dye that absorbs the radioluminescence to produce oxygen-dependent phosphorescence. X-ray excited spectra of our sensor showed ~8 times increase in an intensity at under deoxygenation.

Poster #49

Enhance Electrical and Structural Properties of Metal-Organic Frameworks through Doping Conducting Polymer and Metal Nanoparticle

Weikang Zhang (a), Johnathan Cromer (a), Amina Khatun (a), Monica A. Gordillo (a), Shiyu Zhang (a), and Sourav Saha (a)
(a) Department of Chemistry



Metal-organic frameworks (MOFs) are a class of porous compounds that use the concept of reticular chemistry. Owing to their diverse potentials to help advance modern electronics and energy technologies, electrically conducting MOFs have emerged as one of the most coveted functional materials within the past decade. However, it's quite challenging to design and synthesize intrinsically conducting MOFs in a predictable manner because insulating metal-cluster nodes made of ionic coordination bonds and large spatial separation between the ligands hinder through-bond and through-space charge movement. An effective strategy to address these challenges is to exploit MOF's porosity to introduce appropriate guest molecules, such as conductive polymers (CP) and metal nanoparticles (MNP), to facilitate long-range charge movement and thereby boost their electrical conductivity. Herein, we report three electrically conducting MOF/CP and MOF/CP/MNP composites which utilized this strategy and displayed higher conductivities.

First, we have converted a structurally robust and porous but intrinsically insulating Zn-dpzNDI MOF based on an electron deficient dipyrazolate-naphthalenediimide (dpzNDI) ligand into electrically conducting MOF⊃conducting-polymer (MOF⊃CP) composites via oxidative polymerization of preloaded redox-active 3,4-ethylenedioxythiophene (EDOT) and pyrrole (Py) monomers to corresponding PEDOT and PPy polymers. After monomer loading and in-situ polymerization, the resulting MOF⊃CP composites remained crystalline and displayed significantly higher electrical conductivity (Zn-

dpzNDI⊃PEDOT: 1.8×10-5S/m; Zn-dpzNDI ⊃PPy: 2.5×10-3S/m), whereas the pristine MOF had immeasurably low conductivity (σ < 10-12S/m).1

Second, a highly porous but intrinsically insulating NU-1000 MOF was converted into semiconducting NU-1000/gold nanoparticle (AuNP) and NU-1000/polydopamine/AuNP composites via MOF- and polymer-induced reduction of infiltrated Au3+ ions into metallic AuNPs. The NU-1000/AuNP and NU-1000/PDA/AuNP composites not only gained significant room temperature electrical conductivity (~10-7S/cm), but also retained sizable porosity and surface areas (1527 and 715 m2/g, respectively).2

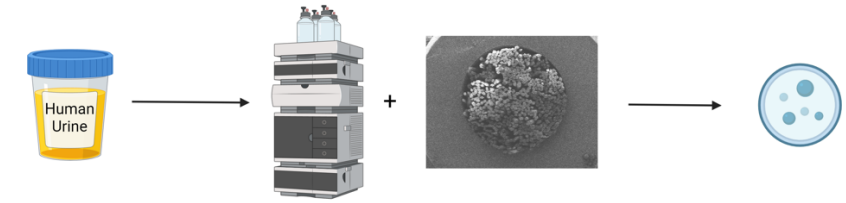
Third, we demonstrate for the first time that the in-situ oxidative polymerization of preloaded EDOT monomers into the PEDOT polymer inside the hexagonal cavities of an intrinsically insulating MOF-74 analogue, which easily collapses and become amorphous upon drying. The resulting PEDOT@Ni2(NDISA) composites displayed improved structural stability, crystallinity, porosity, and electrical conductivity (~10-4 S/cm) compared to the pristine Ni-MOF-74 ((~10-10 S/cm).3

In conclusion, our works presents an effective new strategy to boost the electrical conductivity of intrinsically insulating MOFs by introducing small amount of conducting polymers which provide charge carriers and charge transport pathways.

Poster #50

Isolation of Urinary Exosomes via Hydrophobic Interaction Chromatography using a Nylon-6, Capillary-Channeled Polymer-Based Column

William Pons (a), and R. Kenneth Marcus (a)
(a) Department of Chemistry, Clemson University



Exosomes, a small subset of extracellular vesicles ranging in size from 30-150 nm, are of biomedical interest both for diagnostic testing and therapeutics. These vesicles are excreted from all cell types and thus are found in numerous biofluids such as urine, blood, saliva, etc. More importantly, the vesicles contain important biomarkers that reflect the characteristics of their host cells. Before they can be used in medical applications, exosomes need to be isolated from the biofluid. However, due to the small size of exosomes, isolation is a challenge and can involve very long separation times (ultracentrifugation) or impure eluates (size exclusion chromatography, polymer-based precipitation). Herein, a hydrophobic interaction chromatography (HIC) based separation was paired with a nylon-6 capillary-channeled polymer (C-CP) column to separate exosomes from human urine. Due to the highly hydrophobic nature of exosomes, HIC can successfully separate exosomes from less hydrophobic biofluid matrix contaminants (salts, sugars, proteins). A step gradient approach was used, where a high ionic strength loading condition increases binding affinity for hydrophobic species; subsequent steps remove salt and apply organic modifier, allowing separation of proteins from exosomes. Previous studies by Marcus and colleagues have used a polyester (PET) based C-CP column for exosome separations. However, nylon-6 shows potential for increased isolation efficiency, including greater column loading capacity and a decreased concentration of organic modifier for exosome elution. Another advantage over previous PET columns is that ion exchange modalities can be more easily applied to nylon-6 columns due to intrinsic amine and carboxyl groups in the fiber makeup. The efficacy of this approach has been supported by Bradford assays, transmission electron microscopy (TEM), and flow cytometry. Bradford assays confirmed that protein concentrations in the exosome eluate have been significantly reduced (~4-fold). TEM was used to confirm that isolated vesicles were of the correct morphology. The NanoFCM Flow Nanoanalyzer was used to measure the number density, distribution of vesicles in the eluate, and provided immunoconfirmation using FITC-labeled CD81 antibodies. Overall, this approach utilized a low-cost (~$5) and time-efficient (~15 min) C-CP fiber-based column to yield urinary exosomes of high purity required for downstream techniques, including diagnostic testing and therapeutics.

Poster #51

Lateral Flow Assay Noninvasively Read Through Tissue Using X-ray Excited Luminescence Chemical Imaging

Yu Ding (a), K. Bradley Kelly (b), Morgan N. Reel (a), Matthew J. Case (c), and Jeffery Anker (a)

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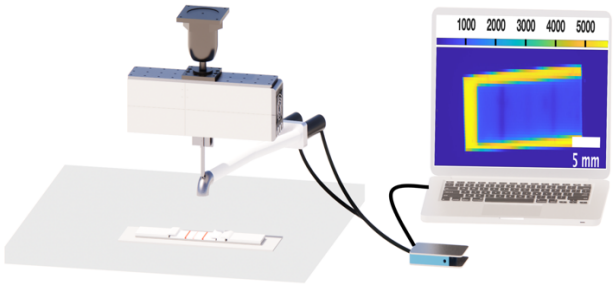

Lateral flow assays (LFAs) are simple point-of-care devices which can be exposed to a bodily fluid and rapidly generate a line if analyte is present. They are widely used in pregnancy tests and to detect infectious diseases; they are also used to detect C-reactive Protein which is a synovial fluid biomarker for prosthetic joint infection. Implanting a lateral flow assay (or smaller version) in a tissue of interest (e.g., joint to detect infection, or tumor to study progression) has not previously been tried likely because one would need to start the assay on command, and more importantly would need to read a small optically absorbing line through tissue. We address the first concern by sealing the LFA with wax, which only opens when activated with ultrasound. We address the second problem using X-ray Excited Luminescence chemical imaging (XELCI), which is a non-invasive technique and provides high spatial resolution images through thick tissue. We used a polycapillary lens to focus the x-ray source and let the beam penetrates the tissue without much scattering, then it will irradiate to the scintillator layer which is composed of scintillator particles. This scintillator layer could be excited by the x-ray and emit luminescence that could be absorbed by the LFAs in different intensity. After the dilutions of the C-reactive protein and use LFA test kits to run different concentrations, the intensity of test lines could be obtained. The different intensity of the test lines will affect the how much light will be absorbed by the test lines. Then, the light will be collected by an in-house machined acrylic light guide and directed to a splitter which will transmit the light to two photomultiplier tubes (PMTs) that one will pass 620nm light and the other pass 700nm light. Finally, each PMT connects with a Data Acquisition (DAQ) board and a program called LabVIEW will record PMT counts and display an image on the computer screen during acquisition. We also use the XELCI to image the different intensity of the LFAs with 6 mm pork tissue. According to the obtained raw data from XELCI, the images could be analyzed by MATLAB and find the intensity of test line and control line.

Poster #52

Developing Rapid test for Neisseria Gonorrhea Bacteria in Patient Urine Sample

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Department of Chemistry, Clemson University

We are developing a rapid test for detecting gonorrhea bacteria in patients' urine samples. Neisseria gonorrhea is a human pathogen that is the second most common sexually transmitted infection in the US. According to WHO estimates, there are approximately 87 million new infections yearly. Unfortunately, the infections are sometimes asymptomatic and can spread very fast. This infection is a leading cause of pelvic inflammatory disease and infertility. The current method for detecting Neisseria gonorrhea bacteria in urine samples is to apply nucleic acid amplification tests (NAAT), which are unsuitable for point-of-care testing. Cell culturing tests are time-consuming. In this research, we aimed to develop a rapid and sensitive test for detecting Neisseria gonorrhea bacteria.

Our technique includes utilizing 15-um microbubbles and magnetic beads with specific antibodies targeting the outer membrane protein of bacteria. Microbubbles and magnetic beads will form a complex with bacteria; this complex is visible to the camera in the setup. Microbubbles offer a higher capture rate quickly because of their large surface area. Their buoyancy enhances their mobility so that they can capture the analyte quickly. With these characteristics, microbubbles improve mass transfer in the test liquid sample. The fast capture rate and simple, portable test setup make it suitable for point-of-care applications.

This assay demonstrated high sensitivity in a shorter time than other existing techniques. This technique provides fast and efficient gonorrhea screening in different healthcare settings, even with minimum equipment, helping to prevent the spread of Neisseria gonorrhea infections.