2026 East Alabama / West Georgia ACS Local Section Research Symposium
List of Abstracts

Oral Presentations – Room 102

9:40-10:00
Title: Detection of Structural Characterization of Alzheimer's Disease Biomarkers using Multidimensional Ion Mobility Mass Spectrometry

Presenting Authors: Kim Kartoworikomo (Graduate Student) – Auburn University

Abstract: Alzheimer's disease (AD) is a progressive neurodegenerative disorder and the sixth leading cause of death in the U.S., with no cure and only treatments that slow the progression. This creates a strong need for rapid, reliable, and cost effective diagnostic methods. Current approaches are often invasive, slow, or lack molecular specificity, and the structural complexity of AD related biomarkers makes them difficult to analyze with conventional tools. LC-IM-MS/MS adds an orthogonal separation based on molecular size, shape, and charge. This presentation introduces a multidimensional, multi omics LC IM MS/MS workflow to improve structural characterization of lipidomic and proteomic biomarkers, aiming to enhance diagnostic precision and biological understanding. LC IM MS/MS methods were developed and optimized for lipidomic and proteomic biomarker analysis. Lipid standards from porcine brain extracts and protein standards were used to support method validation. Proteins were examined using top down and bottom up workflows with tryptic digestion. Biomarker standards were spiked into biologically relevant matrices, including CSF, to imitate AD samples. The optimized methods were applied to mouse brain tissue and CSF from AD and non AD cohorts. Lipids, metabolites, and proteins were extracted and analyzed using optimized methods, followed by data processing using MassHunter software, Skyline, UniDec, and a custom Python pipeline for feature extraction and statistical analysis.

Ion mobility separations uncovered extensive isomeric and conformational heterogeneity not resolvable by LC or MS alone. For example, GT1b (36:1) exhibited multiple IM-resolved features corresponding to distinct ceramide compositions, confirmed by diagnostic MS/MS fragment ions. Similar structural complexity was observed for phospholipids, particularly PE, PS, and PC classes, where multiple LC and IM peaks with unique fragmentation patterns indicated the presence of isomers. Application of the optimized LC-IM-MS/MS workflows to AD and non-AD mouse brain tissues enabled clear discrimination using principal component analysis and machine Learning statistical approaches in both positive and negative ion modes. Furthermore, phosphatidylserine PS (41:7) displayed distinct IM profiles across healthy female and male, AD male, and AD female samples despite identical LC retention times, highlighting the added discriminatory power of ion mobility. Proteomic analysis of intact amyloid peptides demonstrated substantial conformational heterogeneity. A-1-40 and A-1-42 resulted in multiple partially resolved IM peaks at the same charge states, even when LC and MS/MS results indicated a single structural compound. The peptide LQTAPVPMPDLK from bottom-up analysis of tau-441 revealed two distinct IM features, indicating conformers or isomers inaccessible through LC and MS/MS separations alone. These findings highlight that IM provides critical structural information.

In parallel, a Python-based machine learning workflow was developed to extract and preserve multidimensional LC-IM-MS/MS features, enabling robust statistical analysis while maintaining inter-parameter correlation integrity. For example, MS relative intensity profiles were consistent with those visualized using IM-MS Browser. Collectively, these results demonstrate that LC-IM-MS/MS enables high-confidence structural characterization and disease-state discrimination of AD biomarkers. Integration of LC-IM-MS/MS multi-omics workflows with advanced data analysis can resolve structural heterogeneity in Alzheimer's Disease biomarkers.

10:00-10:20
Title: Programmable Lab-on-a-Chip Systems using Valve Actuated 3D-Printed Microfluidic Devices for Biological Applications

Presenting Author: Sabita Dangol (Graduate Student) – Auburn University

Abstract: Microfluidic methods have permitted new insights into biological systems, for example, by allowing microscale cell and tissue co-culture and organ-on-a-chip applications. Our research group has been nearly working for two decades to apply microfluidics to quantitative, dynamic analysis of glycerol and non-esterified free fatty acids (NEFA) released from white adipose tissue (WAT). These devices have achieved high temporal resolution using droplet-based microfluidics. However, fabrication and operation of these systems remain mostly limited to device experts. Fortunately, 3D-printing for microfluidic device fabrication has emerged as a significant alternative to traditional fabrication in the past few years due to its cost effectiveness, capability for direct 3D modeling, and time efficiency through rapid device iterations. Exploiting the benefits of 3D-printed devices for microfluidics, our group aims to adapt prior microfluidic systems into 3D-printed versions to enable non-experts to use the technology. In this work, we move toward this goal by developing Arduino controlled, valve-based, 3D-printed microfluidic modular stimulation devices as well as a programmable droplet generator showing their potential application in biological systems. The stimulation device includes a normally closed pneumatic valve control layer and a separately printed flow layer sandwiching a 0.5 mm PDMS membrane for valving. The droplet device has inlets for the aqueous phase and droplet-dispersing oil phase, a T-junction for droplet generation, and an outlet which uses only a handheld syringe. All valves were Arduino controlled using solenoid-actuated vacuum, and fluid could be pumped using a three-valve membrane pump design or a one-valve pump. Stimulation devices have been validated through imaging and adipose tissue experiments, and programmable droplet devices have been shown functional by creating trains of 64 droplet with a well-defined binary code pattern. We plan to optimize and further automate these inexpensive, 3D-printed devices to use them to study the dynamics of adipose tissue undergoing valve-switched stimulation as well as though well protected droplets of nanoliter (nL) volumes.

10:20-10:40

Title: Discrimination of Foodborne Bacterial Pathogens using Liquid Chromatography Ion Mobility Tandem Mass Spectrometry (LC-IM-MS/MS)

Presenting Author: Iffat Jerrin (Graduate Student) – Auburn University

Abstract: Foodborne illness remains a major public health challenge worldwide and is primarily caused by the consumption of food contaminated with harmful microorganisms. According to the World Health Organization (WHO), approximately 10% of the global population suffers from foodborne diseases each year, resulting in more than 420,000 deaths. Despite significant advances in food manufacturing practices and safety regulations, foodborne disease outbreaks continue to occur, highlighting the urgent need for accurate and sensitive detection methods for foodborne pathogens. Although a wide range of microorganisms can cause foodborne illnesses, most of those cases and fatalities are attributed to bacterial species such as Campylobacter, Escherichia coli, Salmonella enterica, and Listeria monocytogenes. Previous studies have demonstrated the potential of differentiating bacterial species and strains based on their cellular lipid profiles using liquid chromatography-ion mobility-mass spectrometry (LC-IM-MS/MS). This presentation discusses our efforts in developing an accurate detection method for differentiating major bacterial serotypes associated with foodborne illnesses. Two complementary approaches were employed: lipid analysis from individual bacterial cultures and from co-culture samples. Nine bacterial serotypes from three different species were cultured in Luria broth and the lipids were subsequently extracted using a solid-phase extraction method and analyzed using our optimized workflow. Lipid identification was performed using a Personal Compound Database and Library generated through an extensive literature survey. Multiple lipid classes, including PGs, PEs, CLs, lysyl-PGs, DAGs, and DGDGs, were identified and confirmed based on exact mass, isotopic abundance, collision cross-section values, and fragmentation patterns. When combined with principal component analysis (PCA), this platform overcame several limitations of conventional analytical techniques.

10:50-11:10
Title: DNA melting at electrode surfaces to study biosensor stability with square-wave voltammetry (SWV)

Presenting Author: Ugonna D. Nwankpa (Graduate Student) – Auburn University

Abstract: DNA-based biosensors have proven invaluable in medical diagnostics, especially in significantly reducing testing turn-around time and increasing sensitivity. Many biosensors utilize DNA interaction with other biomolecules such as antibodies due to DNA's high hybridization fidelity and antibody-antigen's binding specificity. Our group developed the bowtie biosensor using analyte-tagged DNA based on the reduction of its tethered diffusion upon binding of an antibody. The bowtie sensor is fabricated by enzymatically ligating three DNA strands: the thiol DNA which immobilizes the entire strand on a gold-on-glass (GoG) electrode, the analyte-tagged anchor DNA to which the antibody binds, and the methylene blue DNA which serves as a redox reporter. These strands hybridize to form a bowtie-shaped structure with 14 and 15 base pairs, meltable regions that are intermolecular. Ligation turns the structure into a continuous surface-tethered strand with 19 and 20 base pairs, respectively, in a much more stable intermolecular hairpin configuration. These base pair differences, and particularly the surface tethering, should affect the stability of the sensors to heat and their ability rehybridize after exposure to water. In the present study, ligated and non-ligated bowtie biosensors were subjected to increasing heat treatments to determine their melting temperatures (Tm) and to water rinses to determine their rehybridization ability. Current measurements were collected using SWV. The results show that ligation increased the Tm from 55 °C to above 75 °C. However, both ligated and non-ligated sensors were stable to buffer and water rinses. These results help to confirm the integrity and structure of the Bowtie biosensor and open the way for further improvement of the sensor's sensitivity and other performance characteristics.

11:10-11:30
Title: Comprehensive Discrimination of Foodborne Bacteria Using Whole-Omics Profiling by LC-IM-MS/MS in Combination with Machine Learning Algorithms

Presenting Author: Adebowale Oyerinde (Postdoc) – Auburn University

Abstract: Foodborne pathogens are a major cause of gastrointestinal illness, posing serious risks to public health and generating substantial economic losses. Conventional microbiological detection methods are limited by long turnaround times and insufficient discriminatory power, which can delay clinical decision-making and appropriate treatment. We previously showed that the integration of ion mobility with liquid chromatography-mass spectrometry (LC-IM-MS) enhances analytical sensitivity and resolving power, enabling improved separation of isomeric and conformational molecules and facilitating bacterial identification at the strain and sub-strain levels. In this study, we developed an LC-IM-MS-based whole-omics platform integrating lipidomics, proteomics, and metabolomics, coupled with machine-learning algorithms, for accurate identification of foodborne pathogens. The approach was applied to single cultures, co-cultures, and mixed analyses of multiple bacterial species and their respective strains, including Bacillus, Salmonella, Campylobacter, Clostridium, Escherichia coli, Shigella, Yersinia enterocolitica, and Listeria monocytogenes. Our results demonstrated that the whole-omics approach can effectively differentiate foodborne pathogens, providing novel insights and enabling real-time diagnostics of foodborne pathogens.

11:30-11:50
Title: Improving ion transmission across the Funnelâ€“SLIM interface through SIMION simulations with experimental validation

Presenting Author: Viraj Gandi (Postdoc) – Auburn University

Abstract: Ion mobility spectrometry (IMS) has proven to be a potent method for analysis of complex molecular mixtures by providing quasi-orthogonal separation to mass spectrometry. As modern IMS platforms achieve increasingly high resolving power, overall performance is often limited not by separation within the mobility region, but by ion transmission efficiency into IMS, which directly reduces sensitivity. In this work, we investigate ion injection from an ion funnel into a drift-tube-based Structures for Lossless Ion Manipulation (SLIM) device across an interface gap upstream of the mobility region using both simulations and experiments. The system operates at 4 Torr, with ions exiting the funnel through a 2.5 mm diameter aperture and entering SLIM. Ion trajectories across this interface were studied using the SIMION simulation software package. We have utilized electric fields to explain the observed ion transmission differences as a function of the spacing gap between the funnel exit and SLIM entrance. Moreover, experimental measurements using a standalone funnel-SLIM platform confirmed the simulation trends, with ion transmission increasing at higher gap fields. A resolving power of approximately 27 was achieved at an axial field of 10.41 V/cm and 45 cm long SLIM, while arrival times and resolving power remained unchanged across gap field conditions, demonstrating that improved ion injection can be achieved without compromising mobility performance.

Oral Presentations – Room 108

9:40-10:00
Title: Benchmarking Foundational Models for High-Throughput Exfoliation-Energy Screening of MAX Phases

Presenting Author: Md. Aminul Islam (Graduate Student) – Tuskegee University

Abstract: Prediction of exfoliation energies in MAX phases is critical for guiding the discovery of high-quality MXenes, although using traditional Density Functional Theory (DFT) to accurately predict such behaviors on large compositional spaces is still computationally expensive. In this work, I benchmark the Universal Model of Atoms (UMA) and Message Passing Atomic Cluster Expansion (MACE) potential for calculating exfoliation energies of MAX phases. The calculations are done with the UMA-S-1.1 model in the Meta-FAIRChem framework and MACE model for a chemically broad set of nine group elements (Al, Si, P, Ga, Ge, As, In, Si, Sb and Sn) with nine transition metal (Ti, Zr, Hf, V, Nb, Ta, Cr, Mo and W) compositions. The findings reveal that UMA reliably reproduces the structural and energetic trends for carbide MAX phases, but yields less favorable energies for nitride systems. UMA performs more poorly than MACE. Both models furnish stable energy profiles for exfoliation conditions. This work demonstrates that foundational models are a computationally cost-effective method for high-throughput screening of MAX phases and guiding the Mxene-related research.

10:00-10:20
Title: Engineering superparamagnetic iron oxide nanoparticles (SPIONs) for contrast-enhanced MRI

Presenting Author: Zainab Olowewe (Graduate Student) – Auburn University

Abstract: Superparamagnetic iron oxide nanoparticles (SPIONs) have emerged as promising MRI contrast agents owing to their high magnetic susceptibility, intrinsic biocompatibility, and biodegradability. Despite these advantages, conventional SPIONs predominantly act as Tâ,, contrast agents, producing negative (dark) contrast that can obscure anatomical details and complicate the distinction between healthy and diseased tissues. Therefore, developing ultrasmall SPIONs (â‰¤ 10 nm) with tunable surface or environmental modifications that promote Tâ,⍰-weighted contrast behavior offers a safer and more diagnostically effective alternative to conventional agents.
In this study, we investigate the contrast property of Polyethylene glycol modified SPIONs (PEG-SPIONs). By tuning SPION core size and surface coating thickness, we evaluate their influence on the longitudinal (Tâ,⍰) and transverse (Tâ,,) relaxation times of surrounding water protons. The synthesized SPIONs were stabilized with poly (acrylic acid) (PAA) to prevent aggregation and characterized using Dynamic light scattering (DLS) and zeta potential measurements, confirming a narrow size distribution and good colloidal stability.

Structural analyses (XRD, FTIR, and TGA) are being conducted to confirm the crystalline structure, surface functional groups and presence of polymer coatings on both bare and PEG-modified particles. Ongoing work focuses on evaluating how these relevant surface parameters affect the relaxometry behavior of SPIONs, with the goal of developing a controllable strategy to fine-tune their contrast efficiency.

Hydrophilic super paramagnetic iron oxide nanoparticles (SPIONs) coated with poly(acrylic acid) (PAA) were synthesized via co-precipitation of iron chloride ions in aqueous solution, following established protocols. SPIONs of varying sizes were achieved by adjusting the PAA amount and were subsequently characterized by their physiochemical properties including particle size, polydispersity index (PDI), and zeta potential using dynamic light scattering (DLS). The functional (-COOH) groups and iron content were quantified using titrimetric analysis and the ferrozine assay respectively .To improve biocompatibility and circulation time, SPIONs are functionalized with poly (ethylene glycol) (PEG) of varying molecular weights (PEG-1000, PEG-2000, PEG-5000) via EDC/NHS coupling, enabling covalent bonding between PAA-COOH groups and PEG-NH2 groups. The efficiency of PEG functionalization will be assessed through measurements of particle size and zeta potential, while PEG content and grafting degree will be quantified using barium iodide and ferrozine assays.

We successfully synthesized SPIONs of small and uniform sizes, exhibiting good colloidal stability as confirmed by their measured physiochemical properties. The intensity weighted size distribution shows a narrow and uniform particle distribution with an average hydrodynamic diameter of ~12nm. This small hydrodynamic size suggests that the particle core diameter is likely â‰¤ 10 nm. The low PDI (0.148) indicates a monodisperse nanoparticle suspension with minimal aggregation in aqueous media. Additionally, the negative zeta potential value is consistent with the presence of surface carboxylate groups from the poly (acrylic acid) coating, which contributes to electrostatic stabilization of the colloid. Ongoing PEG functionalization and relaxometry studies will further elucidate how surface modification influences stability, magnetic properties and contrast efficiency properties of SPIONs. These results are expected to inform the rational design of SPION-based T1 contrast agents with improved safety and diagnostic performance.

10:20-10:40
Title: Insights into the Electronic Structure of $(\text{Ti-CO}_2)^-$ and $(\text{V-CO}_2)^-$ Species

Presenting Author: Alexandros Androutsopoulos (Graduate Student) – Auburn University

Abstract: It is widely recognized that CO_2 capture and utilization is important for both environmental and economic reasons. On the one hand, the reduction of CO_2 promotes a neutral carbon cycle, while on the other hand, atmospheric CO_2 practically provides an infinite source of carbon. The ground electronic state of CO_2 is a highly stable closed-shell singlet with zero dipole moment and negative electron affinity. That is, CO_2 anion lies higher in energy than neutral CO_2. Thus, both capture and utilization processes are particularly challenging. Our group recently explored the potential of transition-metal anions for solving such a "chemistry enigma" by introducing molecular catalysts featuring electron-rich metals (CERMAs). The first step of this "computational journey" is to examine the interaction between a bare metal anion and CO_2 in the gas phase. Within this context, our study focuses on providing accurate mechanistic insights and energetics for the reaction between titanium/vanadium anions and carbon dioxide using density functional theory and high-level ab initio methods. To the best of our knowledge, such a fundamental theoretical study is missing from the literature.

10:50-11:10

Title: Ab Initio Design of 2D Electrides with Hybrid Electronic Structures

Presenting Author: Andrei Evdokimov – grad – auburn – computational

Abstract: Solvated Electron Precursors (SEPs) - are metal-ligand complexes with peripheral diffuse electrons with unique pseudoatomic electronic structures, determining their intriguing properties in quantum computing and CO_2 capture and utilization. SEPs serve as building units of expanded metals and organic electrides, however their possible applications and synthesizability are hindered due to structure complexity and stability issues. Here we present a novel family of electrides, where SEP molecules are anchored to passivated surfaces which we term Surface Immobilized Solvated Electron Precursor Electrides or SISEPEs. The adsorption of molecular species to the stable substrates is a well-known approach that helps to achieve synthesizability of desired material. By tuning the coverage density of SEPs on the surface, the electronic structure of SISEPEs can be varied from isolated delocalized electrons to one-dimensional electronic channels and two-dimensional 'seas' of electrons. The tunability of electronic structures is intriguing, as it allows to switch between organic-electrides-like electronic structures (0D and 1D) and inorganic-electrides-like electronic structures (2D), maintaining the same chemical composition. Hence SISEPEs can be referred to as hybrid organic/inorganic electrides. We also demonstrate the impact of the substrate on the electron transfer from SEPs to the bulk of material by investigating both diamond and silicon carbide based SISEPEs. The electron affinity of the surface plays a major role in this process, further diversifying the tunability of SEP-based materials. In this study we utilized periodic plane-wave DFT simulations using r2scan hybrid functional implemented in VASP software. To support these results, we performed gas-phase simulations using CAM-B3LYP hybrid DFT functional implemented in Gaussian 16 package to study the kinetical stability of SEPs anchored to the surfaces with respect to H2 release reaction.

11:10-11:30
Title: Exploring the adsorptions properties of Thiophene on Bimetallic Surfaces

Presenting Author: Melvin Emioma (Undergraduate Student) – Tuskegee University

Abstract: We present a density functional theory (DFT) of thiophene (SC4H4) adsorbed on five different bimetallic (100) surfaces with the aim of evaluating these materials and their properties as hydrodesulfurization (HDS) catalysts. We utilize the optB88-vdW functional, which includes a correction to include long range dispersion, for our calculations. To find the active site, we screen ten different adsorption sites over these bimetallic surfaces. We present both the adsorption energy, adsorption height, buckling of the surfaces, and charge transfer to the S atom as calculated with the Badger charge analysis program. Furthermore, using a previously described relationship between HDS rate, adsorption energy, and charge transfer to the S atom, we then predict the HDS rate of the sulfurized version of these materials using charge transfer to the S atom and adsorption energy.

11:30-11:50
Title: Effects of polymer side chains on ultrafast dynamics of electrochemically induced polarons.

Presenting Authors: Zainab Adeoluwa (Graduate Student) – Auburn University

Abstract: Conjugated polymers (CPs) are widely studied for use in modern organic electronic devices due to their tunable conductive properties. They exhibit electrical and optical properties owing to their conjugated backbone which allows the transport of charges. CP charge transport can be fine-tuned by electrochemical doping (oxidation or reduction) which creates a mobile charge carrier known as polaron that hops through the backbone of the polymer. To improve charge transport, structural engineering is typically used to control molecular ordering, electronic delocalization, and ionic-electronic coupling. The effectiveness of charge transport in CPs relies on several interactions such as molecular ordering, electronic delocalization, and ionic-electronic coupling. While several studies have explored the impact of side chains on crystallinity and conductivity properties through various spectroscopic techniques, the specific role of side chain engineering in optimizing these properties is yet to be understood. In this study, we are studying the effect of including an extra methyl group in the side chain of a model polythiophene system (P3MEEET and P3MEEMT) by using transient absorption-spectroelectrochemistry. We observed polaronic features in the near-infrared spectrum upon electrochemical oxidation of both polymers. However, at low bias only P3MEEET formed ion-free polarons, suggesting that its more ordered structure (due to its larger side chain) enhances polaron mobility by preventing ion-trapping. At higher bias, ion-bound polarons are primarily formed in the disordered phase in both polymers, where the ions can electrostatically trap polarons. These findings suggest that polymer structure can be exploited to increase the amount of ion-free polarons to improve conductivity at low bias, which could improve their performance in electrochemical devices.

Oral Presentations – Room 202

9:40-10:00
Title: Blue Light Enabled C-C Bond Cleavage in Heteroarene Dimers. Dearomative Alkylation of Heteroarenium Salts.

Presenting Author: Agshin Garayev – grad – auburn – organic

Abstract: Nitrogen heterocycles are a common motive in bioactive compounds. Dearomatization of heteroarenes is an efficient strategy towards synthesis of substituted nonaromatic heterocycles. This work presents a method for dearomatization of nitrogen heterocycles via cross electrophile coupling. The method uses N-alkyl salts and alkyl halides as coupling partners. Wide variety of substrates are explored. Mechanistic studies are performed to understand the nature of the reactivity.

10:00-10:20
Title: Design of Alkynylated [6]CPPs for Strain-Tolerant π-Extension Reactions

Presenting Author: Taiwo Adepoju (Graduate Student) – Auburn University

Abstract: The structural extension of [n]cycloparaphenylenes (CPPs) into larger π-systems remains a significant synthetic challenge. Conventional oxidative Scholl reactions, while powerful for planar polycyclic aromatic hydrocarbons, are poorly suited for CPP π-extension due to strain sensitivity, uncontrolled over-oxidation, and limited regioselectivity. To address these limitations, we report the design and synthesis of an alkynylated [6]CPP as a tailored substrate for controlled Ï€-extension via iodine monochloride (ICl)-mediated annulation. This strategy enables selective intramolecular cyclization under mild conditions, avoiding the harsh oxidative environment characteristic of Scholl chemistry. The ICl-mediated annulation provides an efficient and modular route to radially π-extended CPP architectures, offering improved structural control and functional group tolerance. This work establishes alkynylated CPPs as versatile platforms for strain-compatible Ï€-extension and expands the synthetic toolbox for constructing curved nanocarbon fragments relevant to nanographenes and carbon nanotube end-caps.

10:20-10:40
Title: Chelating bisCAAC–Cu Carbene Complex: Synthesis, Characterization, and Preliminary Reactivity

Presenting Author: Chase Ledbetter (Graduate Student) – Auburn University

Abstract: Chelating bis(cyclic)(alkyl)(amino)carbene (bisCAAC) ligands offer exceptional ?-donation and tunable sterics, but their practical use is often limited by counterion effects, fleeting free-carbene behavior, and hard-to-reproduce metalation outcomes. We report a workflow that converts a di-iminium bisCAAC precursor into a reliably metalated Cu(I) platform by combining anion management (iodide ? BF??/BArF?), controlled deprotonation conditions, and rapid trapping with soluble Cu sources. Across multiple Cu salts (Cl?, I?, OTf?, BF??, BArF?), the Cu–carbene resonance is consistently observed near ~247 ppm in ^{13}C NMR, supporting a convergent Cu–bisCAAC solution species in which the anion is largely outer-sphere under the conditions examined. Early reactivity tests and UV–vis titrations show the Cu–bisCAAC complex is remarkably resistant to coordination or oxidation in donor solvents like MeCN, so current efforts are shifting toward less competitive media and ligand/anion tuning to access isolable, crystallography-ready derivatives. Ongoing work targets structurally definitive Cu–bisCAAC complexes and simple, diagnostic reactivity that connect solution speciation to isolability and downstream behavior.

10:50-11:10
Title: Manganese Complexes with a Fluxional Bipyridine Backbone Enabling Multi-Electron Energy Storage in Redox Flow Batteries

Presenting Author: Charles Daramola (Graduate Student) – Auburn University

Abstract: Grid-scale energy storage through redox flow batteries (RFBs) is critical for addressing the growing global demand for reliable electricity and mitigating risks of electricity famine. Stable and efficient redox-active electrolytes capable of storing excess solar and wind energy are urgently needed. This research focuses on first-row coordination compounds that exhibit a concerted 2-electron redox feature, effectively doubling energy storage capacity. We report a series of Mn(bpyR)(CO)3X complexes featuring bipyridine ligands substituted at the 6- or 6,6'-positions. These fluxional ligands adapt structurally during redox cycling, enabling smooth transitions through intermediate oxidation states (Mn(I) to Mn(-I)) and leveraging disproportionation to establish a robust 2-electron redox couple governed by metal-ligand bond formation. Continuous charge-discharge cycling demonstrates more negative redox potential and improved capacity retention in the presence of excess bromide ion, thereby improving the performance of Mn complexes as anolytes in RFBs. This work highlights a promising pathway for optimizing multi-electron energy storage systems through ligand design, offering new directions for next-generation energy storage systems.

11:10-11:30
Title: Zinc enhanced $2e^-$ redox chemistry for Ni(IV/II) diethyldithiocarbamate couple

Presenting Author: Smriti Somai (Graduate Student) – Auburn University

Abstract: Redox Flow Batteries (RFBs) are excellent candidates for grid scale applications because they are easily upscaled and are safer to use than commercially available Lithium-Ion Batteries (LIBs). However, current RFBs have lower energy density than LIBs. Multi-electron redox chemistry of molecules at a single potential can be leveraged to increase the energy density of RFBs. Nickel(II) N,N-diethyldithiocarbamate (Ni(II)(dtc)2) undergoes two-electron (2e-) ligand coupled electron transfer to [Ni(IV)(dtc)3]+ upon oxidation and reforms Ni(II)(dtc)2 when reduced. Cyclic Voltammetry (CV) experiments in MeCN/TBAPF6 show a single 2e- oxidation wave while the reduction displays two sequential 1e- waves. The anodic process occurs through an ECE-DISP 1 mechanism where E is electron transfer step, C is chemical step and DISP is disproportionation. In contrast, the cathodic process was found to occur through an EEC mechanism. The addition of zinc salts causes the reduction waves to combine into a single 2e- reduction wave changing the mechanism to ECE where the chemical step is catalyzed by Zn(II)ions. Zinc salts used in this study are Zn(ClO4)2, Zn(BF4)2, ZnCl2, ZnBr2, Zn(NO3)2 and Zn(OTf)2. While all Zn salts were found to enhance 2e- behavior, there are differences in the rate of the chemical step due to coordination geometry around the Zn(II) ion. CV and square-wave voltammetry (SWV) were used to study the electrochemical mechanisms. Nuclear Magnetic Resonance (NMR) and UV/Vis spectroscopy were used to study the binding of zinc salts to the nickel complex. ZnCl2 was found to have the weakest binding to Ni(II)(dtc)2 because of strongly coordinating Cl- ions and slowest rate constant for chemical step. However, strongest binding was observed for Zn(NO3)2. ZnBF4 was found to have the fastest rate constant for the chemical step. Adding Zn(II) salts also affected the anodic wave by forming an encounter complex causing a second oxidation peak to be observed. This work highlights the key role of the chemical step in facilitating the overall 2e- Ni(IV/II) redox cycle and shows that Zn(II)ions are able to serve as catalysts in both the oxidation and reduction directions.

11:30-11:50

Title: Concerted two-electron renewable energy storage for redox flow batteries by nickel bis(diphosphine) complexes

Presenting Author: Md Musharraf Hossain (Graduate Student) – Auburn University

Abstract: The unique architecture of redox flow batteries (RFBs), which can decouple energy density from power density, has encouraged scientists to consider them a promising renewable energy storage system for grid scale applications due to their safety, cost-effectiveness, and durability. In RFBs, redox-active molecules are used to store and release energy as anolytes and catholytes in solutions. The energy stored ($\Delta G = -nFE_{cell}$) depends on the number of electrons (n) transferred per molecule and the potential difference between catholyte potential (E_c) and anolyte potential (E_a) where $E_{cell} = E_c - E_a$. Increasing energy density and finding redox-active molecules of high stability are the two main challenges for practical use of RFBs. The storage of multiple electrons per molecule can greatly enhance the energy density of RFBs. Here, we studied that easily synthesized, highly stable Ni(dppe)2(BF4)2, where dppe = 1,2-bis(diphenylphosphino)ethane, efficiently store multiple electrons through sequential 1e- redox waves. Mechanistic studies have been shown that coordination of monodentate ligands (e.g., $X^- = Cl^-$, Br^-) allow for selective control of the electron transfer pathway, steering electron storage toward the more favorable concerted 2e- redox wave. We also found that addition of quantitative dppe ligands creates new electron transfer pathway and further improves single potential 2e- reversibility and shows excellent charge-discharge cycling stability as anolyte in energy storage RFBs. This work shows how mechanistic understanding of 2e- redox cycles for transition metal complexes can create new opportunities for multi-electron storage in RFBs.

Oral Presentations – Room 208

9:40-10:00
Title: Conductive Biodegradable PBAT/PHB Polymer Nanocomposites

Presenting Author: Aboulfazl Barati (Faculty) – Troy University

Abstract: Conductive biodegradable polymer nanocomposites are emerging as sustainable alternatives to conventional conductive plastics for applications ranging from biomedical devices to flexible electronics and sensors. In this work, conductive nanocomposites were developed based on blends of poly(butylene adipate-co-terephthalate) (PBAT) and poly(hydroxybutyrate) (PHB). The polymers were melt-blended using a twin-screw extruder (Process 11) to achieve homogeneous mixing and scalable processing. PBAT provided ductility and toughness, while PHB contributed stiffness and bio-based content. Carbon-based conductive nanofillers were incorporated to impart electrical conductivity while maintaining biodegradability. The effects of blend composition and nanofiller loading on melt processability, viscoelastic behavior, and electrical performance were examined. The resulting PBAT/PHB nanocomposites exhibited improved flexibility compared to neat PHB and demonstrated stable conductive pathways suitable for multifunctional applications. These results highlight the potential of PBAT/PHB-based conductive nanocomposites as sustainable materials for next-generation functional polymer systems.

10:00-10:20
Title: Life Cycle Assessment of an Optimized Carbon Dioxide Capture Process in a Pulp and Paper Mill

Presenting Author: Chukwuma Nwanazoba (Graduate Student) – Auburn University

Abstract: The pulp and paper industry is energy-intensive and ranks fourth globally in energy consumption. Globally, the United States pulp and paper industry is the second largest, with a production of 72 million tons of paper and paperboard in 2022 and an average of 942 kg of CO_2 emitted for every ton of paper produced. The Kraft pulping process accounts for approximately 73% of all papermaking processes in the US. However, there is no existing CO_2 capture unit in any of the Kraft pulp mills in the US. The limited adoption of CO_2 capture and utilization in the pulp and paper industry is primarily due to the high energy requirements of the process, which affect capture costs. Furthermore, the CO_2 emissions from the pulp and paper industry are largely biogenic and thus excluded from CO_2 emission regulations. The capture of these CO_2 emissions can move the Kraft pulp and paper industry forward towards achieving carbon neutrality, which is its unique potential compared to other industries. Moreover, the CO_2 captured in the industry has various utilization options internally for tall oil manufacture, lignin separation, production of precipitated calcium carbonate (PCC), brown stock washing, near-neutral bleaching, and pH control for stock preparation. Additionally, the captured CO_2 can be used to produce bio-derived plastics, carbon-neutral fuels, and a range of other chemicals. A comprehensive analysis of these applications has been explored by Gulzar et al.

Our previous research on techno-economic optimization of CO_2 capture has demonstrated the economic feasibility of an optimized CO_2 capture process for the pulp and paper industry. The results from the optimized process were used in this work to evaluate its environmental impact. A cradle-to-gate life cycle analysis (LCA) was performed using the openLCA software with the ecoinvent database. Three CO_2 capture processes were modeled in Aspen Plus v15 for three capture configurations involving flue gas emissions from the bark boiler (BB), the recovery boiler (RB), and the limekiln (LK), which are the three major emission sources in the pulp and paper industry. The material flows and utility requirements (electricity, steam, and cooling water) for each of these configurations were used to carry out the LCA.

The system boundary for the analyses encompassed the three sections: the dehydration section, where the flue gas temperature was reduced and 99% of its water content removed; the capture section, where CO_2 was removed from the flue gas stream; and the compression section, where the captured CO_2 is compressed and liquefied for transportation and utilization. For each of these processes, two case scenarios were explored: the base case, in which the emitted flue gas is discharged freely without capture (Scenario 1), and the emitted flue gas is processed to capture CO_2 using the optimized capture process (Scenario 2). A functional unit of 1 kg of captured CO_2 was used to compare the environmental impact of the three capture configurations. The environmental impact assessment methods used to analyze the results were the Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) version 2.1 and the Intergovernmental Panel on Climate Change (IPCC) 2013. The impact categories covered by TRACI include Acidification, Climate change, Ecotoxicity (freshwater), Eutrophication, Human toxicity (carcinogenic and non-carcinogenic), Ozone depletion, Particulate matter formation, and Photochemical oxidant formation. The IPCC covers global temperature change and global warming potentials over 20- and 100-year periods.

The TRACI results showed significant impacts on climate change, freshwater ecotoxicity, and eutrophication, while others were negligible. For these significant impact categories, Scenario 2 had a lower (negative) impact on climate change and eutrophication, whereas Scenario 1 had a higher (positive) impact. This was corroborated by IPCC analysis, which showed all negative values for Scenario 2 and positive values for Scenario 1. In each of these results, the recovery boiler exhibits the largest reduction, due to its higher flue gas emissions than the bark boiler and limekiln. However, Scenario 2 had a significant impact on freshwater ecotoxicity, attributable to the raw materials and utilities used in the capture process. Analysis of the capture process based on the functional unit (1 kg of captured

CO_2) showed that the environmental impact of capture from the bark boiler, recovery boiler, and lime kiln was similar.

Future work will explore the environmental impact of combined capture from these sources. An additional assessment will explore the environmental impact of an improved capture process involving process intensification or the use of alternative capture solvents. This will ensure economic feasibility by reducing energy consumption while maintaining a low environmental impact. The tradeoff between process efficiency and environmental compatibility will also be explored in detail. To this end, further analysis of the contributions of raw materials and utilities to each impact assessment category will be conducted.

10:20-10:40
Title: Lead ion removal from aqueous solutions using biochar materials from different wood species

Presenting Author: Ruiqi Li (Graduate Student) – Auburn University

Abstract: The increasing severity of heavy metal contamination in water resources is driven by industrialization and urbanization. It is necessary to develop efficient remediation methods to reduce heavy metal bioavailability and mobility. Biochar has emerged as a promising adsorbent due to its unique physicochemical properties, including high surface area, abundant surface functional groups, and inorganic mineral content. However, the performance of biochar in heavy metal adsorption varies significantly depending on the feedstock. This study investigated the influence of feedstock on lead ion adsorption by characterizing the physicochemical properties and lead ion adsorption capacities of twelve woody biochar materials. Results revealed that lead ion adsorption capacity was primarily governed by biochar pH, EC, and mineral content (e.g., calcium carbonate). In contrast, parameters such as specific surface area, elemental composition, and porosity exhibited limited correlation with adsorption efficiency. These findings highlight the critical role of feedstock selection in customizing biochar to enhance heavy metal remediation. This study provides actionable insights for designing cost-effective, feedstock-specific biochar to address lead contamination in aquatic environments.

10:50-11:10
Title: Survey of Volatility and Polarity of Hazardous Volatile Organic Compounds (VOCs) Potentially Present in Recycled Plastics

Presenting Authors: Chloe Higdon, Julie Le Bras (Undergraduate Students) – Troy University

Abstract: Recycled plastics may contain hazardous volatile organic compounds (VOCs) that can affect product quality and pose potential human health risks. In our prior work, 622 potential contaminants reported or anticipated in recycled plastics were screened using NFPA health ratings and identified 366 chemicals with NFPA health ratings of 2 or more. Here, we evaluate the volatility and polarity of these 366 potentially hazardous contaminants to support development of a comprehensive solid-phase microextraction (SPME)-GC/MS analytical method. Key properties indicative of volatility (melting point, boiling point, flash point, and vapor pressure) and polarity (octanol-water partition coefficient, logP) were collected from credible sources, including government-supported databases and major chemical manufacturers. The results reveal substantial diversity in both volatility and polarity. Boiling points span from below 0 Â°C to above 350 Â°C, while room-temperature vapor pressures range from greater than 100 to less than 1.0 Ã— 10-6 mm Hg. LogP values range from less than 0 (highly polar) to over 10 (highly nonpolar). These results demonstrate that hazardous VOCs potentially present in recycled plastics occupy a broad volatility-polarity space, indicating the need for an analytical method which is capable of capturing compounds across wide physicochemical ranges. The property analysis provides foundational guidance for designing a more comprehensive SPME-GC/MS workflow to monitor VOCs associated with elevated health concerns in recycled plastics.

11:10-11:30

Title: Physicochemical and Microstructural Characterization of Zeinâ€“Chitosan Macro-Polyelectrolyte Complexes (Macro-PECs)

Presenting Authors: Camila Ridrigues Carneiro (Graduate Student) – Auburn University

Abstract: Polyelectrolyte complexes (PECs) formed by biopolymers, such as proteins and polysaccharides, have attracted increasing scientific and technological interest due to their techno-functional relevance, particularly in the food, cosmetic, and bioremediation sectors. Protein-polysaccharide complexation can be influenced by pH, biopolymer mass ratio, and temperature. In this study, zein (ZN) and chitosan (CHS) sized at the millimeter scale (namely macro-PECs) were obtained by mixing dispersions of both biopolymers at different pH (4.1, 5.1, or 7.1), ZN:CHS mass ratios (1:2, 1:1, or 2:1), and temperatures (25 °C or 45 °C) combinations. The systems were characterized in terms of visual inspection, Tyndall effect, zeta potential, electrophoretic, macro-PECs gravimetric yield, scanning electron microscopy (SEM), and Brunauer-Emmett-Teller (BET) specific surface area (SSA). Among all conditions evaluated, regardless of temperature or ZN:CHS ratio only at pH 7.1 there was formation of macro-PECs, resulting in sharp phase separation with suspended macro-PECs particles and a low turbidity supernatant. At this pH, yields were 80%. The macro-PECs exhibited slightly negative zeta-potentials, indicating effective electrostatic contributions to the macro-PECs formation, as zeta-potentials of separated ZN and CHS in aqueous dispersions were respectively -15 mV and +10 mV. These macro-PECs displayed aggregated microstructures with rough surfaces, microcavities, and irregular fissures. Complexes obtained with mass ratio ZN:CHS = 2:1 showed the highest specific surface area (5 m^2 g^{-1}). These results demonstrate that ZN-CHS macro-PECs can be efficiently produced under simple mixing conditions in aqueous media, using low quantities of organic solvents and without crosslinkers. These supramolecular structures are now being investigated by our research group in terms of their applicability for encapsulation and controlled release of small bioactive molecules, as well as pollutants adsorption.

Poster Abstracts

Poster 1

Title: Janus Liposomes: Exploring Liquid-Liquid Phase-Separating Lipid Systems Alternative to DOPC/DPPC/Cholesterol

Presenting Author: Ayesha Akter (Graduate Student) – Auburn University

Abstract: Existing work on Janus liposomes almost exclusively employs the ternary lipid system based on 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC), 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC), and cholesterol (Chol), offering limited material choice, stability, and operating temperature window. In this work, we have systematically investigated >30 binary/ternary lipid combinations as potential alternatives to DOPC/DPPC/Chol to produce microsized Janus liposomes. A variety of structural/chemical differentiators are explored to induce phase separation in these systems, such as chain length (C10 to C18), unsaturation level (1 to 3 double bonds per acyl chain) and headgroup identity (phosphatidylcholine, phosphatidylglycerol and sphingomyelin). Using confocal fluorescence microscopy, we have identified eight new Chol containing systems that produce Janus liposomes indecent to high yields. Furthermore, we also discover that global liquid-liquid phase separation can occur within individual Chol-free, binary liposomes, despite at much lower yields compared to Chol-containing systems. Evaluating these successful cases together with other tested systems, we also attempt to provide a set of guidelines for designing and preparing phase-separated liposomes. These findings may be of value to workers in membrane biophysics, particularly related to lipid liquid-liquid phase separation, as well as those interested in exploring Janus liposomes as an anisotropic colloidal material, for example, in liposomal drug delivery and active matter.

Poster 2

Title: Dielectrophoretic Motion and Assembly of Janus Liposomes

Presenting Author: Debneela Paul (Graduate Student) – Auburn University

Abstract: Liquid-liquid phase separation in cell membranes has been increasingly recognized as a general guiding principle in cellular organization and functions, to which lipid systems with well-defined phase relationships continue to serve as useful models to decipher the structure and dynamics involved. However, direct experimental strategies that can non-invasively probe the dielectric and interfacial properties of coexisting membrane phases under dynamic electric fields remain limited. In this work, we subject microsized liposomes in either liquid-ordered or liquid-disordered phases, or in coexistence under AC dielectrophoresis, and quantitatively resolve their field-driven motion and assembly, phase-dependent polarization, and dielectric response using fluorescence microscopy. Several salient trends have emerged from this systematic investigation, including liposome accumulation, pearl-chain formation, size-based sorting, levitation, reversible shape transitions, self-rotation, and phase-specific alignment perpendicular to the applied electric field. These unique liposome responses arise within discrete, frequency-dependent windows across the AC spectrum tested (10 Hzâ€“30 MHz). Together, these results demonstrate dielectrophoresis as a mechanistically informative platform for resolving phase-dependent interfacial dielectric properties in heterogeneous lipid membranes under dynamic electric fields, providing a quantitative framework for interrogating membrane phase coexistence and electrostatic heterogeneity.

Poster 3

Title: Advances in method development to achieve reusability of a DNA-based electrochemical bowtie sensor integrating physical and chemical means

Presenting Author: Eloge Lwamba (Graduate Student) – Auburn University

Abstract: The electrochemical bowtie sensor is a DNA-based structure designed for generalizable detection based on its modularity and adaptability to multiple types of analytes. Next to demonstrating robustness in assay readout conducted in 95% human serum for creatine kinase, the bowtie sensor's versatility in detecting both large proteins and small molecules is an added advantage. This work aims at making the sensor reusable, a feature that would make it stand out even more. The high-affinity interaction this probe has with its target antibody has made its regeneration toward reuse unsuccessful despite using conventional trials with an IgG immunoaffinity buffer, along with other chemical approaches. Recently, a physical approach based on potential variation at the electrode has been considered, a method developed by the Kelley group termed â€œactive reset.â€� To attempt active reset with our bowtie sensors, we chose to modify the voltage waveform (Gamry Reference 600 potentiostat) from the typical square wave voltammetry (SWV) to achieve rapid oscillations with only a very small potential scanning window. The hypothesis was that the negatively charged DNA strands in the bowtie sensor would quickly oscillate by switching the potential fast enough between positive and negative ranges to induce the antibody unbinding. Using a bowtie sensor with a testosterone-DNA conjugate, we have applied our active reset method in tandem with a high concentration of competing free testosterone, and this has shown a possible route to reverse the binding. However, the effects have been minimal to date. Optimizing this approach could result in a fully automated technique that would require microfluidic device integration for rapid free testosterone introduction between assay runs. Alternatively, the system could be explored with lower-affinity sensor components to explore the efficiency of the developed SWV approach to remove the target antibody, as a way of validating the technique.

Poster 4

Title: A novel probe for sensitivity enhancement of DNA monolayer-based electrochemical sensors

Presenting Author: Mainul Islam Mazumder (Graduate Student) – Auburn University

Abstract: Detecting biomarkers is vital for diagnosing diseases, tracking disease progress, and evaluating treatment effectiveness. Common methods for biomarker detection are often slow and labor-intensive. DNA monolayer-based electrochemical sensors are promising for point-of-care diagnosis because they respond quickly, are easy to miniaturize, and provide real-time monitoring. However, measuring biomarkers within clinically relevant ranges remains a challenge. Typically, a methylene blue (MB) molecule attached to single-stranded DNA (MB-DNA) serves as a redox reporter in these sensors and is highly effective. Other redox-active molecules have also been used, but MB is preferred due to its stable potential window. Still, improving signal strength is necessary for higher sensitivity. In this study, we show a significantly increased sensitivity of DNA monolayer sensors using a novel probe design. One of our sensor platforms is termed the “bowtie sensor” which features an on-electrode (2D gold-on-glass) attachment of thiolated DNA (thio-DNA), analyte-conjugated DNA, and MB-tagged DNA (MB-DNA). We modified the MB-DNA in these sensors and compared them to unmodified versions, observing a 4-6 fold increase in current with the same configuration. We also used these sensors to detect estradiol, testosterone, and progesterone, improving detection limits from the nano- to pico-molar ranges. Additionally, a similar signal enhancement was seen when this modified redox reporter was attached to a vancomycin aptamer sensor. This approach significantly boosts the sensitivity of aptamer-based electrochemical sensors, enabling operation in nanomolar ranges. Interestingly, this modified redox reporter increases electrical signals even at low square wave voltammetry (SWV) frequencies, allowing enhanced faradaic current and further decreased nonfaradaic current. This method reduces reliance on pulse techniques like SWV. For the electrochemical bowtie sensors, we were able to collect 252 nA of faradaic current alongside only 3 nA of nonfaradaic current at 10 Hz SWV frequency. These findings indicate that chronoamperometry with delayed sampling times can replace SWV for electrode interrogation. A custom-built potentiostat could be a more cost-effective alternative with engineered temporal responsiveness for these sensors. Since our redox reporter is MB-based, the redox potential window minimizes monolayer degradation, enhancing the sensor’s durability.

Poster 5

Title: Lipidomic-Based Identification of Five Salmonella Serovars Using Liquid Chromatography Ion Mobility Mass Spectrometry (LC-IM-MS/MS)

Presenting Author: Md Naymor Rahaman (Graduate Student) – Auburn University

Abstract: Pathogenic Salmonella are major foodborne pathogens responsible for significant numbers of hospitalizations and deaths worldwide. Rapid and accurate identification and discrimination of Salmonella serovars are therefore critical for effective clinical management and for minimizing public health risks. Traditional microbiological methods generally find it difficult to accurately discriminate between the serovars due to the high degree of phenotypic and antigenic similarity among them. However, a multidimensional separation workflow provided through ion mobility coupled with liquid chromatography and tandem mass spectrometry (LC-IM-MS/MS) enables the discrimination of the biomarkers. Here, we used LC-IM-MS/MS for accurate identification of five Salmonella serovars. Bacterial samples were cultured in Luria Broth (LB) medium for 16 hours at 37Â°C with shaking, and lipids were extracted using the Folch method. Numerical multivariate statistical analysis, including principal component analysis (PCA) followed by linear discriminant analysis (LDA), was performed to validate the capability of this method to achieve high-level discrimination. Interestingly, preliminary analysis of the LC-IM-MS/MS data revealed several lipid isomers and conformers, enabling discrimination among Salmonella serovars. This highlights the potential of this approach for clinical diagnostics and public health surveillance.

Poster 6
Title: Surface-Specific and Bulk Measurements of Aerosol Acidity

Presenting Author: Sheba Maaji (Graduate Student) – Auburn University

Abstract: Acidity strongly influences atmospheric chemistry, affecting heterogeneous reaction kinetics, aerosol composition, cloud formation, and pollutant lifetimes. Many atmospherically relevant processes occur at the surface of aerosols, where acidity can differ significantly from the bulk phase. In this work, we use second harmonic generation (SHG) spectroscopy, a surface-specific nonlinear optical technique, to probe interfacial acidity. Crystal violet and DiA4 serve as molecular pH-sensitive probes, enabling quantification of interfacial protonation states. Surface-specific and bulk measurements of aerosol pH are compared, and implications for atmospheric chemistry are discussed.

Poster 7
Title: On-Liposome Click Reaction

Presenting Author: Sanju Maharjan (Graduate Student) – Auburn University

Abstract: Copper-catalyzed azide-alkyne cycloaddition (CuAAC) or “Click” reaction is fast, simple, and gives significant yield. However, Click reactions in biological systems encounter challenges such as copper toxicity, limited surface accessibility of azide and alkyne groups, stability concerns, and complex lipid environments. In this study, we aimed to develop a straightforward and readily adoptable on-liposome Click reaction procedure with optimal amounts of catalyst, reactant, ligand, and reducing agent. For the first time, this important conjugation strategy will be applied to phase-separated lipid systems such as PSM/DOPC/cholesterol. Specifically, the liposomes will be modified in such a way that it labels only the disordered liquid lipid phase with Rhodamine-DOPE. This approach will open a new pathway for modifying or incorporating different agents onto the liposome surface, enabling selective and targeted drug delivery in a simple and efficient manner.

Poster 8

Title: Characterization of Secondary Organic Aerosol Physicochemical Properties via Fluorescence Probe Spectroscopy

Presenting Author: Michael Boadu (Graduate Student) – Auburn University

Abstract: Secondary organic aerosol (SOA) physicochemical properties such as hygroscopicity, degree of oxidation, phase state, pH, and viscosity influence important processes that ultimately impact air quality and climate. Due in part to the experimental challenge of in situ characterization, these physicochemical properties remain incompletely understood. Here, an aerosol fluorescent labeling methodology in conjunction with a fluorescence aerosol flow tube (F-AFT) was used for in situ physicochemical characterization of Î±-pinene and toluene SOA. The wavelength of maximum emission Î»max of the fluorescent probe Prodan was shown to depend on the hygroscopicity, degree of oxidation, and relative humidity (RH)-dependent phase transitions of the SOA. At varying RH, Î»max was shown to be linearly correlated with % water content. For fixed RH and varying SOA oxidation conditions, the Î»max was linearly correlated with the SOA oxygen-to-carbon ratio (O:C). Finally, the Î»max of mixed toluene SOA/ammonium sulfate particles indicated that these mixed particles were liquid-liquid phase separated within RH range of 40 to 80 %RH. Overall, these results demonstrate the power and versatility of this approach for direct, online physicochemical analysis of SOA.

Poster 9

Title: In Situ Single Particle Measurements of Submicron Aerosol Particle Phase State

Presenting Author: Vincent K. Kipter (Graduate Student) – Auburn University

Abstract: Aerosols in plays an important role in atmospheric processes affecting air quality, human health, and climate, including virus transmission, and cloud activation. Atmospheric aerosols are inherently heterogeneous, with particle-to-particle variability in composition and morphology that cannot be fully captured by ensemble-averaged measurements. Consequently, resolving aerosol phase and mixing state requires physicochemical characterization at the single-particle level. These properties include, phase state, pH, hygroscopicity and viscosity. In situ measurements of aerosol properties for individual particles remain experimentally challenging due to their small size, low mass, and their dynamic behaviour. Fluorescence-based techniques employing environmentally sensitive probes have recently emerged as promising tools for probing aerosol microenvironments. Excited-state intramolecular proton transfer (ESIPT) fluorophores, in particular, 2-(2-benzofuranyl)-3-hydroxychromone (3-HC) exhibit large Stokes shifts and strong sensitive to polarity and hydrogen-bonding interactions, making it well suited for probing aerosol phase state. However, ESIPT-based approaches have thus far been largely limited to ensemble aerosol measurements. Here, we present the development of an in situ single-particle aerosol spectroscopy technique that enables direct, non destructive, particle-resolved measurements of phase state at the submicron scale of mixed organic and inorganic systems using ESIPT fluorescence probing. In this approach, 3-HC is volatilized and incorporated into atomized polyethylene glycol and NaCl aerosol particles, with phase transitions studied over a range of relative humidities. This approach provides access to aerosol phase and mixing state heterogeneity under atmospherically relevant conditions, offering new insight into aerosol physicochemical behaviour that is inaccessible through bulk measurements.

Poster 10
Title: Characterization of Metal-Linked Diisocyanide Self-Assembled Monolayers under Electrochemical Control by SFG-Stark Spectroscopy

Presenting Author: Celestine Egemba (Graduate Student) – Auburn University

Abstract: Controlling molecular behavior and reactivity at interfaces remains one of the fundamental challenges in surface chemistry. Applying an external electric field offers an effective approach to modulate interfacial structure and function, enabling the design of responsive and selective surfaces. In this work, self-assembled monolayers (SAMs) of diisocyanides linked by ruthenium coordination on gold are examined under electrochemical control using sum-frequency generation (SFG)-Stark spectroscopy. The vibrational Stark response reveals a clear, linear correlation between applied potential (-0.6 to +0.2V vs Ag/Ag+) and the interfacial CN stretching frequency, demonstrating that molecular dipoles directly sense and respond to local electric fields within the stable potential window. This field-dependent behavior establishes SFG-Stark spectroscopy as a sensitive probe for mapping electric-field effects at metal-organic interfaces. Future studies will extend this approach to other d-transition metal complexes to establish systematic structure-field response relationships, guiding the rational design of adaptive catalysts for controlled interfacial reactivity.

Poster 11
Title: Fluorescence behavior of probe molecules in model aerosol constituents

Presenting Author: Victoria Cover (Undergraduate Student) – Auburn University

Abstract: The transmission of respiratory viruses via aerosols is impacted by environmental factors such as temperature and relative humidity, which alter the physicochemical properties of the aerosols. A mechanistic understanding of these impacts requires in situ measurements of these physicochemical properties, which remain challenging. Fluorescence measurements coupled with a polarity-sensitive fluorescent probe is one of the few techniques capable of in situ measurements of the phase state of aerosols. However, accurate inferences from a fluorescent probe require a comprehensive understanding of probe molecule behavior in aerosol chemical environments, which are typically characterized by very high salt concentrations. Here absorbance and fluorescence measurements of Nile red and Prodan in organic/inorganic model aerosol environments are presented. Additionally, quantum yield results are presented to compare the efficacy of both probes in these solutions. The outlook of using Nile red and Prodan for future studies of aerosol physicochemical properties is then discussed.

Poster 12

Title: Does ligand-induced signaling by ERBB4 heterodimers drive BRAF-WT melanomas?

Presenting Author: David J. Riese II (Faculty) – Auburn University

Abstract: Melanomas that possess wild-type BRAF alleles ("BRAF-WT melanomas") are less responsive to targeted therapies and immune checkpoint inhibitors than melanomas that possess gain-of-function mutant BRAF alleles. Thus, identifying the genetics of BRAF-WT melanoma to be translated into significant advances in the treatment of these tumors. We will present population and reverse genetics data suggesting that ERBB4 heterodimers drive BRAF-WT melanomas. We will also present our attempts to translate these results into small-molecule inhibitor approaches for treating BRAF-WT melanomas.

Poster 13

Title: Heterologous expression of Hydroxylase MMOH protein of Soluble Methane Monooxygenase (sMMO) from Methylosinus trichosporium OB3b (Mt OB3b)

Presenting Author: Harun Abdullah (Graduate Student) – Auburn University

Abstract: Soluble methane monooxygenase (sMMO) enables methanotrophic bacteria to eat methane as their only source of carbon and energy. sMMO from Mt OB3b is a multicomponent metalloenzyme with the remarkable ability to break the strong C-H bond in methane, which has a bond dissociation energy of 105 kcal/mol, and incorporate one oxygen atom from O2 to produce methanol under mild conditions without overoxidation.1 sMMO consists of three unique components: hydroxylase MMOH (comprising Î±, Î^{2}, and Î^{3} subunits), reductase MMOR, and regulatory MMOB.2 This enzyme can co-oxidize over 50 hydrocarbon substrates, including aromatic and non-polar aliphatic compounds.3 Its promiscuous nature has suggested many potential applications in biocatalysis, biotechnology, and bioremediation. Heterologous expression of the non-heme diiron active site hydroxylase MMOH component outside the native organism has been a long-standing challenge due to its structural complexities and the difficulty in achieving the proper folding of this component in non-methanotrophic hosts. This challenge has limited simple modifications of the MMOH protein, which are essential for understanding the roles of various second- and third-sphere amino acid residues involved in sMMO reactivity and regulation. Functional expression of sMMO from Methylococcus capsulatus Bath (Mc Bath) has been reported in E. coli by co-expressing sMMO with its cognate GroEL/ES-like chaperone, MMOG.4 Additionally, both MMOG and MMOD have been demonstrated to play a crucial role in the assembly and activity of sMMO from Methylotuvimicrobium buryatense 5GB1C. In this study, we attempted to co-express the MMOG GroEL/ES-like chaperone from Mc Bath, along with MMOH (mmoX, mmoY, and mmoZ) and MMOD (mmoD) from Mt OB3b, in E. coli.5 Protein characterization using SDS-PAGE gels showed soluble expression of the Î±, Î², and Î³ subunits (MMOH) in equal stoichiometric amounts with and without co-expression in E.coli. Future work will focus on purifying and evaluating the enzymatic activity of the heterologously expressed MMOH in E. coli.

Poster 14

Title: Activation Complex of Methyl-Coenzyme M Reductase (MCR)

Presenting Author: Thach Do (Graduate Student) – Auburn University

Abstract: Methane plays a dual role as both a critical driver of global climate change and a significant energy resource. Biologically, its production and consumption are governed by a specialized enzyme known as Methyl-coenzyme M reductase (MCR), which is a dimer of heterotrimers composed of McrA (Î±), McrB (Î²), and McrG (Î³) subunits. This enzyme depends on a unique nickel-containing coenzyme F430 in the active site and several unusual post-translational modifications (PTMs) that influence its catalytic efficiency and stability. The structure of the methyl-coenzyme M reductase (MCR) activation complex is a sophisticated multi-protein assembly designed to overcome the significant energy barrier of reducing the enzyme's nickel-containing cofactor, F430, from Ni(II) to its active Ni(I) state, EÂ°â€²â€‰=â€‰âˆ’650â€‰mV. From previous studies, activation complex (mentioned as A3a complex in the literature) was able to be purified from the native methanogen strains and Ni (II) state was able to reduce to NI(I) state, but the measure activity of MCR is only roughly around 1% of the expected activity. A hypothesis was made that since the complex is a large, multi-protein assembly (A3a), essential proteins or subunits are frequently lost during traditional multi-step purification procedures. Similarly, from the cryo-EM paper, only a small amount of activity of MCR was seen, one possibility is that the complex presented in the structure is still incomplete and still missing some of the catalytic subunits. Recombinant activation complex of MCR is proposed to solve the issue. A well-understood process of maturation and activation of MCR can lead to a new application for natural gas conversion (renewable energy) and also reduce the greenhouse gas emission which could lead to global warming.

Poster 15

Title: Towards identifying the role of a cytochrome P450 (CYP107) protein in the bacillaene biosynthetic gene cluster (BGC)

Presenting Author: Kwansima Nana Adjoa Quansah (Graduate Student) – Auburn University

Abstract: Secondary metabolites are low-molecular-weight bioactive compounds that afford the microorganisms that produce them advantages over ecological competitors.

Biosynthetic gene clusters (BGCs) are a set of contiguous genes that encode the production of specific secondary metabolites. A hallmark of species from the bacterial genus Bacillus is their prolific production of secondary metabolites with potentially valuable properties (e.g., antibiosis, plant growth stimulation, etc.). Within some Bacillus BGCs, cytochromes P450 have been identified. In other contexts, these enzymes are known as key tailoring enzymes that catalyze otherwise challenging redox transformations. Despite their prevalence in these BGCs, their roles remain unassigned.

In this study, we evaluate the function of a cytochrome P450 (CYP107) identified in the BGC of a Bacillus-based metabolite, bacillaene, and its reduced form, dihydrobacillaene. Bacillaene is a highly unsaturated linear polyene assembled by a hybrid type I polyketide synthaseâ€“nonribosomal peptide synthetase (PKS-NRPS) pathway. Our studies have revealed that the relative abundance of these two closely related isoforms varies within culture parameters such as growth hours, growth medium, dissolved oxygen ratios, temperature, and agitation rates. Based on the redox chemistry for which P450s are known, we hypothesize that this CYP107 catalyzes the dehydrogenation of dihydrobacillaene to generate bacillaene. Further, we propose that this oxidative transformation generates a metabolite (bacillaene) with greater antimicrobial potency and/or range than dihydrobacillaene.

Capitalizing on complete genome sequence for B. velezensis strain JJ334, we assigned this P450 to the CYP107 family and generated a clone for heterologous expression of the gene in E. coli. We have successfully expressed and purified this enzyme in a soluble heme-containing state. Evaluation of the product by SDS-PAGE and UV-visible spectroscopy revealed that a protein of the anticipated molecular weight and bearing a P450-like heme spectrum had been isolated. A molar absorptivity for this P450-bound heme was determined. We compared the conversion of one isoform to the other using both the peroxidase shunt pathway and the NADPH-dependent redox conditions in the presence of a redox partner. The P450-mediated reaction was monitored by HPLC, LC-MS, and UV-visible spectroscopy. Also, both the substrate and the product were evaluated for antibacterial activity against representative Bacillus strains and Escherichia coli to assess how P450-mediated structural modification influences biological activity.

This study seeks to answer questions addressing the role of P450s in Bacillus BGCs and link structural modification of metabolites to microbial competition and plant pathogen control.

Poster 16

Title: Exploring Structure-Function Relationships via Experimental and Computational Methods in Dinoflagellates Bioluminescent

Presenting Author: Joshua D. Ehun (Graduate Student) – Auburn University

Abstract: Dinoflagellates are a major group of eukaryotic microbes found in both freshwater and marine environments. Some species are responsible for harmful red tides and can produce potent toxins that negatively impact human health and coastal ecosystems. Certain dinoflagellates are known for their bioluminescence and photosynthetic capabilities. The bioluminescence process in dinoflagellates occurs when the enzyme luciferase (LCF) catalyzes the oxidation of an open chain tetrapyrrole (luciferin substrate). The activity of the luciferase enzyme is predominantly controlled by pH, where it exhibits minimal activity at pH âˆ¼8, with optimal function occurring at pH âˆ¼6. Here, more emphasis has been placed on the mechanistic studies of LCF from two dinoflagellate species; Lingulaulax polyedra (Lp) and Noctiluca scintillans (Ns). Unlike most dinoflagellates that possess distinct LCF and LBP components (the former typically consists of three homologous catalytic domains encoded within a single polypeptide), Ns-LCF presents a strikingly different organization, where the LCF and LBP exist as a unique fused protein that integrates both enzymatic and substrate-binding functionalities into a single polypeptide chain. Sequence alignment analysis shows that Ns-LCF (LCF-like domain) shares around 56% amino acid identity with corresponding individual domains of Lp LCF. We integrate biochemical approaches with advanced computational methods to elucidate the structure of LCF from diverse dinoflagellate species and to gain insight into the conformational activation mechanisms induced by acidification.

Poster 17

Title: The active-site [4Fe-4S] cluster in the isoprenoid biosynthesis enzyme IspH adopts unexpected redox states during ligand binding and catalysis.

Presenting Author: Evert C. Duin (Faculty) – Auburn University

Abstract: (E)-4-Hydroxy-3-methylbut-2-enyl diphosphate reductase or IspH (formerly known as LytB), catalyzes the terminal step of the bacterial Methylerythritol Phosphate (MEP) pathway for isoprene synthesis. This step converts (E)-4-hydroxy-3-methylbut-2-enyl diphosphate (HMBPP) into one of two possible isomeric products, either isopentenyl diphosphate (IPP) or dimethylallyl diphosphate (DMAPP). This reaction involves the removal of the C4 hydroxyl group of HMBPP and addition of two electrons. IspH contains a [4Fe-4S] cluster in its active site and multiple cluster-based paramagnetic species of uncertain redox and ligation states can be detected after incubation with reductant, addition of a ligand, or during catalysis. To characterize the clusters in these species, 57Fe-labeled samples of IspH were prepared and studied by electron paramagnetic resonance (EPR), 57Fe electron-nuclear double resonance (ENDOR), and MÓ§ssbauer spectroscopies. Notably, this study provides a rarely reported, complete determination of the 57Fe hyperfine tensors for all four Fe ions in a [4Fe-4S] cluster. The resting state of the enzyme (Ox) has a diamagnetic [4Fe-4S]2+ cluster. Reduction generates [4Fe-4S]+ (Red) with both S = 1/2 and S = 3/2 spin ground states. When the reduced enzyme is incubated with substrate, a transient paramagnetic reaction intermediate is detected (Int) which is thought to contain a cluster-bound substrate-derived species. The EPR properties of Int are indicative of a 3+ iron-sulfur cluster oxidation state and MÃ¶ssbauer spectra presented here confirm this. Incubation of reduced enzyme with the product IPP induced yet another paramagnetic [4Fe-4S]+ species (Red+P) with S = 1/2. However, the g-tensor of this state is commonly associated with a 3+ oxidation state, while MÃ¶ssbauer parameters show features typical for 2+ clusters. Implications of these complicated results are discussed.

Poster 18

Title: Utilizing X-ray Absorption Spectroscopy to Study Selenocysteine vs Cysteine Binding by the Mercurial Transport Protein

Presenting Author: Laura P. Hall (Graduate Student) – Auburn University

Abstract: Elemental mercury (Hg(0)) is a global pollutant that can be oxidized to Hg(II) in the atmosphere and deposited into both marine and freshwater ecosystems.1,2 Hg(II) can then be methylated by many different bacteria3 to form methylmercury (MeHg), a neurotoxin that bioaccumulates in fish and humans leading to serious health complications.4 However, other microbials have developed a mercurial resistance pathway that includes proteins such as the periplasmic Hg(II) scavenging protein (MerP), mercurial transport protein (MerT), and Hg(II) reductase enzyme (MerA), which work together to reduce Hg(II) to Hg(0).5,6 MerT is an integral membrane protein that is believed to use a cysteine â€“ cysteine (Cys-Cys) pair to bind Hg(II) from MerP and pass it through the cell membrane to MerA where it is reduced to Hg(0).5 It has recently been discovered that a small population of proteins contain a cysteine â€“ selenocysteine (Cysâ€“Sec) motif, including MerT from Alkaliphilus metalliredigens, that has not been studied in vitro.7 Sec is the 21st amino acid, is much more acidic than its Cys counterpart (pKa 5.3), and is energetically taxing for cells to incorporate.8 This leads to the question: why would a bacterium evolve to contain a Cys-Sec motif rather than the more common Cys-Cys one? Selenium (Se) has a higher binding affinity for Hg(II) than sulfur (S), and could be the reason this evolution has occurred.9 Our goal is to compare A. metalliredigens MerT to Sulfitobacter faviae MerT, a strain similar to AmMerT containing a Cys-Cys motif natively, by using Hg L-edge X-ray absorption spectroscopy to monitor Hg-Se/S binding and fluorescent probe containing proteoliposomes to determine MerT functional changes. By combining these two techniques, we aim to elucidate if functional changes are caused by binding differences of Se and S to Hg(II).

Poster 19

Title: From methane to methanol: A high-energy quantum chemical insight into how being negative can be positive

Presenting Author: Josephn Olaniyan (Graduate Student) – Auburn University

Abstract: Methane is produced in large quantities (natural gas) and can serve as feedstock for commodity chemicals. Activation of the C-H bond of methane is the first step for such chemical processes and is usually the rate-determining step since the C-H bond of methane is one of the strongest C-H chemical bonds. In this study, we examine the possibility of activating methane using metal anionic centers and adamantane porphyrin-like [MO?] cluster. Specifically, we perform CASSCF and MRCI calculations to investigate the reaction of methane with anion (Cu?, Co?, Ag?, Au?, Ir?) while the clusters: ([CuO?], [NiO?], [CoO?]) were studied at DFT. We optimized the geometries of adsorbed species as reactants, transition states, and the various possible intermediates. Our results show that Cu? and Co? can form stable HCuCH3? and HCoCH3? compounds, albeit via high activation barriers, while Ag? and Au? cannot. Interestingly, Ir? formed a much more stable product H4IrC? beyond the HCuCH3? as observed in others. These observations are in agreement with the experimental photoelectron spectra recorded for the products of the studied reactions. Likewise, all the [MO?] clusters activated CH4 and facilitated methanol release, but at varying energy barriers.

Poster 20

Title: Ionization Potentials: A Comparison of Cluster Perturbation Theory and Electron Propagator Theory

Presenting Author: Malachi Kent (Graduate Student) – Auburn University

Abstract: Cluster Perturbation (CP) theory systematically approximates Coupled Cluster (CC) models to increase computational efficiency without sacrificing accuracy. CP theory shows promising results for calculating both ground state and excited state energies(1), however, ionization potentials (IP) have not yet been explored. CP theory introduces the CC parent state Jacobian partitioning and perturbatively adds corrections that approximate the CC target state. In other words, if no perturbative approximations were introduced then these models would be equivalent to the CC target state, or in the case of excitation energies (EE) and ionization potentials (IP) to EE-EOM-CC and IP-EOM-CC, respectively. In deriving the CP series for IPs, a direct comparison can be seen between the new generation intermediately normalized, Hermitized, superoperator metric Electron Propagator Theory (EPT) methods(2). This occurs within the second and third order approximations. The only differences between the methods were the lack of energy dependence in the denominator of CP derived method and the treatment of singles amplitudes. The EPT methods used MÃ¸ller-Plesset amplitude convention, while CP methods used the CP amplitude convention. Energy dependence can be recovered in CP theory through LÃ¶wdinâ€™s partitioning, but only within the 2hp terms. So, a one-to-one comparison can be made between the non-Dyson EPT methods and an iterative IP-CP model. This study introduces a new CP model for IPs, and most importantly evaluates the significance of the self-energy and the singles amplitude treatments for electron binding energy methods against the quantum chemistry gold standard IP-EOM-CCSD.

Poster 21

Title: Quantum Chemical Interpretation of the Electronic Structure of Neptunium(V)-oxo Complexes and their Stability

Presenting Author: Taylor Gregory (Graduate Student) – Auburn University

Abstract: In this study, our goal is to accurately describe the electronic structure and explain the stability of high-oxidation-state neptunium oxo complexes. We begin by performing high-level electronic structural calculations to examine the low-lying excited and ground electronic states of non-ligated neptunium(V) monoxide. Here, we employed multi-reference methods, including static and dynamic electron correlation, to construct potential energy profiles. Scalar and spin-orbit relativistic effects were incorporated using the Douglas-Kroll-Hess and Breit-Pauli Hamiltonian operators, respectively. Motivated by recent studies, we explored ligand effects using and density functional theory methods. We found that an important factor for their stability is the bridging between the coordinated units, and thus, polydentate ligands are necessary. We also found that the type of ligand is important to the stability of the neptunium-oxide center. Our results will be used to determine if neptunium(V)-oxo units can be used as a catalyst for the conversion of methane to methanol.

Poster 22

Title: Performance and Memory Analysis of a Reworked Pythonic Coupled-Cluster Implementation Solving Jacobian Transformations

Presenting Author: Wyn Newton (Undergraduate Student) – Auburn University

Abstract: Python-based implementations of coupled-cluster (CC) theory offer highly accurate electronic structure calculations, but they are often limited by long computation times and large memory requirements due to extensive tensor contractions. In this project, an existing Pythonic CC workflow was reworked to evaluate the time and memory benefits of a new tensor contraction process. The original scheme utilizing opt_einsum was benchmarked and compared to NumPyâ€™s tensordot along the same contraction pathways. The benchmarking was performed for the CC singles-and-doubles Jacobian transformation and the time and memory required were recorded and compared.

Poster 23

Title: Comparing Approximately Renormalized Methods in Cluster Perturbation Theory and Electron Propagator Theory for Ionization Potentials

Presenting Author: Emily Berlin (Undergraduate Student) – Auburn University

Abstract: Coupled Cluster (CC) theory provides a foundational framework in quantum chemistry for incorporating electron correlation to the Hartree-Fock method through exponential parametrization and delivers a size-consistent description of a correlated electronic structure. Equation-of-motion coupled cluster theory is widely regarded as a gold standard for molecular properties like ionization potentials (IP), specifically ionization potentials equation-of-motion coupled cluster theory with single and double excitations (IP-EOM-CCSD) model.1 Cluster Perturbation (CP) theory extends this framework by incorporating the CC Jacobian within the zeroth order approximation to compute these properties at a significantly reduced cost.2 In parallel, Electron Propagator Theory (EPT) provides a Greenâ€™s function approach for calculating electron detachment energies and has demonstrated strong empirical accuracy with comparatively low computational cost. In this study the performance of the third-order ionization potential CP singles and doubles (IP-CPS(D-3)) model for calculating ionization energies are compared to those obtained from IP-EOM-CCSD and established EPT models.3 Emphasis is placed on approximate renormalization schemas within CP theory, which are rigorously derived, and in EPT. The results provide insight into the relative performance of CP and EPT regarding accuracy of ionization energies and attempt to correlate their approximate renormalization methods.

Poster 24

Title: A Biocompatible and Sustainable Method for Keratin Extraction from Poultry Feathers Using N-Acetylcysteine

Presenting Author: Bahareh Mirmashhouri (Postdoc) – Troy University

Abstract: Poultry feathers are produced in very large amounts worldwide and are often treated as waste, even though they are composed of nearly 90% keratin. Keratin is a biodegradable and biocompatible protein with strong potential for use in bioplastics, biomedical materials, and sustainable composites. Keratin needs to be extracted from feather by breaking its disulfide bonds by using sulfur-containing reducing agents. Most existing extraction methods rely on harsh reducing agents, such as sodium sulfide, which are toxic and harsh, weaken the protein by breaking its backbone chain, and limit the use of keratin in environmentally sensitive and biomedical applications. Here we presents a safe and biocompatible approach for keratin extraction based on N-acetylcysteine (NAC) combined with urea under mild conditions (pH 10, 55 Â°C). NAC is a clinically approved pharmaceutical compound and a common dietary supplement that safely breaks disulfide bonds through thiolâ€“disulfide exchange. Using this method, high keratin extraction yields of 80â€“90% were achieved, comparable to conventional sodium sulfide methods, but without toxic byproducts or unpleasant odors. Structural, thermal, mechanical, and rheological characterization such as FTIR, Â^{1}H/Â^{1}Â^{3}C NMR, DSC, TGA, Instron, and rheometer confirmed the keratin backbone remained mostly intact after extraction. Unlike keratin obtained from traditional processes, the NAC-extracted keratin could be directly processed into flexible cast films and hot-pressed sheets. Mechanical testing showed adjustable tensile strength, elongation, and viscoelastic behavior, with the best overall performance observed at 0.5 M NAC and 8.0 M urea. Rheological and water-absorption studies further showed that NAC promotes tighter chain packing and reduced swelling, while urea enables controlled unfolding and good processability. Overall, this study demonstrates that N-acetylcysteine is a safe, effective, and sustainable alternative to conventional reducing agents, enabling the production of strong, flexible, and processable keratin materials suitable for biomedical, packaging, and environmentally friendly material applications.

Poster 25

Title: Manipulation of the Lewis Acid Catalyzed Esterification Mechanism for Metal Oxide Nanoparticle Synthesis

Presenting Author: Megan Henley (Graduate Student) – Auburn University

Abstract: Metal oxide nanoparticles (NPs) are of high interest due to their size-dependent properties which allow for a wide range of applications in emission, absorbance, energy conversion, and energy storage. Cu2O (cuprite) has been successfully synthesized via a slow injection method where a copper oleate precursor solution is slowly injected into hot oleyl alcohol, resulting in simultaneous esterification and -OH transfer mechanisms to produce Cu2O NPs. Upon the addition of a catalytic amount of Ga3+ to the copper oleate precursor, the esterification reaction becomes more efficient, and more Cu2O NPs are produced. By varying the rate of injection and the concentration of the injected Ga3+ catalyzed precursor solution, changes in the onset of NP production and yield can be analyzed through tracking carbonyl peaks corresponding to the precursor solution and ester using ATR-FT-IR spectroscopy. Further analysis of the post-reaction solution by UV-Vis absorbance spectroscopy and the isolated NPs by X-ray diffraction reveals the efficiency and identity of NP product formation. Unravelling the complexities of this reaction mechanism for Cu2O will open the door to explore more complex, novel materials by this Ga3+ catalyzed method.

Poster 26

Title: Structure-Activity Relationships in Quinol tethered Transition Metal Electrocatalysts for Dioxygen Reduction

Presenting Author: Maksuda Parvin (Graduate Student) – Auburn University

Abstract: Quinol-containing polydentate cobalt complexes (Co(II) and Co(III)) are studied as electrocatalysts for the oxygen reduction reaction (ORR) and compared with their iron analogues to assess how ligand structure influences activity and selectivity. Co(II)-H4qp2 primarily facilitates a four-electron reduction to water (H_2O) at higher overpotentials, while Co(II)-H2qp3 follows a two-electron pathway, producing a mix of H_2O and hydrogen peroxide (H_2O_2). Studies reveal that differences in ligand protonation rates significantly influence catalytic turnover and product distribution, indicating control by proton-coupled electron transfer. A similar increase in water selectivity between H2qp3 and H4qp2 was noted for iron complexes with Fe(II)-H4qp2 being 4.4 times more active than Fe(II)-H2qp3. The TOFmax for Fe(II)-H2qp3 is higher than its phenolic analog, while substituting quinols has less effect on Co(II) than on Fe(II) complexes. Additionally, using Co(III)-H2qp3 reduces the effective overpotential without altering activity or product distribution, a trend also observed with Fe(III)-H2qp3. Comparing iron and cobalt complexes reveals that the increase in activity for H4qp2 over H2qp3 is less pronounced for cobalt, with Co(II)-H2qp3 reducing O_2 at a similar rate to Co(II)-H4qp2 under high acid conditions, where O_2 coordination is rate-limiting. Due to the crucial role of quinolic -OH groups in proton-coupled electron transfer (PCET) during ORR, pKa values of the tethered quinols have been determined, along with pH-dependent mapping of PCET redox processes

Poster 27

Title: Possible catalase mimicry of Mn(II), Fe(II), and Zn(II) complexes with a phenolic ligand

Presenting Author: Precious U. Ebereonwu (Graduate Student) – Auburn University

Abstract: Manganese, iron, and zinc complexes with a macrocyclic ligand with two covalently attached quinols (H4qp4) were previously found to functionally mimic catalase. Here, we complex Mn(II), Fe(II), and Zn(II) to an analog of this ligand that has phenols in place of the quinols (H2pp4) to determine whether the ability of the quinol to engage in two-electron redox is essential for the catalytic dismutation of H2O2. We characterize the complexes by NMR, UV/vis, and IR spectroscopies as well as by mass spectrometry and elemental analysis. We also assess the abilities of the complexes to functionally mimic catalase using oxygraphy measurements to follow the production of O2 during catalytic H2O2 disproportionation.

Poster 28

Title: Synthesis and Characterization of a Benzyl-CAAC to Stabilize Low-Valent Metal Centers

Presenting Authors: Hailey Mackie (Undergraduate Student) – Auburn University

Abstract: The goal of this project is to synthesize a cyclic(alkyl)(amino)carbene (CAAC) ligand, with the intent of forming previously unreported metal complexes with Fe(II) and Cu(I) metal centers. CAACs are known for having strong Ï€-accepting and Ïƒ-donating properties which encourage metal coordination with electron rich metal centers. Here a new benzyl-CAAC ligand precursor has been synthesized via the alkylation of a related enamine compound with benzyliodide. The resultant iodide salt has been characterized by 1H-NMR spectroscopy. In addition, metalation attempts are underway using the strong, non-nucleophilic base, potassium hexamethyldisilylazide followed by treatment with an appropriate metal salt. Comparison of metal complexes with this new ligand will be compared to analogous versions in a xylyl-bridged bis- CAAC complex prepared by another member of the group. The overarching aim of this research is to investigate the potential of the metal-CAAC complex in serving as a synthon for low-valent metal-oxo and - nitrido complexes for use in C-H activation.

Poster 29

Title: Metal Ligand Cooperativity Using a Non-Trigonal Phosphorus Center and Cobalt(II) Chloride Complex

Presenting Author: Avery Musick (Undergraduate Student) – Auburn University

Abstract: Metal-ligand cooperativity continues to be widely studied as a strategy to replace precious metal catalysts with more economically and environmentally favorable first-row transition metals such as cobalt. This study explores the synthesis and catalytic application of a novel cobalt complex containing a urea-backboned ligand featuring a non-trigonal phosphorus center. A multistep synthetic pathway was carried out to successfully form a tridentate 3NPurea ligand with a non-trigonal phosphorus center. This was followed by the addition of cobalt(II) chloride to generate paramagnetic cobalt (II) complex. The catalytic activity of this cobalt complex was evaluated through the hydroboration of various aldehydes and ketones using pinacolborane as the borylation source. Optimization studies revealed that a 0.5% catalyst loading at room temperature provided the highest conversion for benzaldehyde. These optimized conditions were subsequently applied to a range of aldehydes and ketones. These results demonstrate the potential of urea-backboned cobalt complexes for catalytic hydroboration reactions. Future efforts will focus on improving the yield of the cobalt complex, enhancing hydroboration efficiency, reducing catalyst loading, and obtaining a crystal structure of the cobalt complex.

Poster 30

Title: Enhancing Biodegradability and Processability of Recycled PET/PHB Blends for Additive Manufacturing Applications

Presenting Author: Aboulfazl Barati (Faculty) – Troy University

Abstract: Recycled poly(ethylene terephthalate) (rPET) offers significant environmental benefits; however, its limited biodegradability and challenging melt processability restrict its use in advanced manufacturing technologies such as additive manufacturing. In this study, rPET was blended with poly(hydroxybutyrate) (PHB) to enhance biodegradability while improving melt processability for extrusion-based fabrication. Polymer blends were prepared using both a batch mixer (Brabender Plasticorder) and a continuous twin-screw extruder (Process 11) to evaluate the influence of processing method on blend homogeneity and rheological behavior. PHB incorporation introduced bio-based content and promoted biodegradable pathways, while melt blending enabled tunable viscoelastic properties suitable for fused filament fabrication (filament 3D printing). The effects of blend composition and processing route on melt flow behavior and material stability were systematically investigated. The results demonstrate that rPET/PHB blends can achieve improved processability compared to neat rPET while advancing sustainability goals, highlighting their potential for use in additive manufacturing and circular polymer applications.

Poster 31

Title: Repurposing Waste Li-Ion Battery Materials for Efficient Catalysts in Methane Dry Reforming: Oxalic Acid Treatment Approach

Presenting Author: Pritam Vitthalrao Dhawale (Graduate Student) – Auburn University

Abstract: The increasing demand for lithium-ion batteries (LIBs) has led to a rise in spent LIBs. The most efficient way to manage them is through material recovery and repurposing for battery manufacturing or energy storage. However, recovered cathode and anode materials often suffer from lower capacity and efficiency due to structural degradation from previous use. Regardless of the recovery techniques used, the traditional approach of recovering individual elements lacks selectivity, leading to impurity-induced defects that degrade electrochemical properties, lifespan, and stability. This study employs a unique single-element recovery approach for lithium (Li)using hydrometallurgy, optimizing the solubility kinetics of Li-ion extraction in aqueous leachate. The objective is to overcome the limitations of traditional recovery methods while precipitating Ni, Co, and Mn from the leachate, making use of the catalytic synergy of Ni and Co as an effective reforming catalyst. A black powder (crushed LIB cathode) is made Li-free by optimizing concentration, time, temperature, and acid medium. The leaching efficiency of Li-compound was analyzed using ICP-OES and confirmed via TGA and XRD. Transition metals (Ni, Co, Mn), precipitated as oxalates through acid leaching, were processed into catalysts via drying, calcination, and Hâ,,-based reduction. Given the challenges of using recovered materials for energy storage applications like grid storage or back-up power systems, methane dry reforming (DRM) offers a promising alternative. DRM was conducted using these recovered metals as catalysts, with syngas (Hâ,,:CO) production monitored via in-line mass spectrometry and optimized using inert gas tuning. The synergistic effect of the multi-metallic catalyst enabled DRM to be carried out at a lower reforming temperature, improving efficiency while reducing energy consumption. This repurposing strategy addresses key DRM challenges by lowering the reforming temperature and catalyst costs. It also mitigates excessive rare earth mining and prevents catalyst coking due to the reduced operating temperature.

Poster 32

Title: Metal-Organic Framework Foam Composites for Next-Generation Filtration Applications

Presenting Author: Jai'Ana Burditte (Undergraduate Student) – Tuskegee University

Abstract: Activated carbon filters are currently the standard for air filtration in military applications due to their high efficiency in adsorbing gases and vapors. However, these filters pose limitations in practicality in dynamic field environments due to their weight, stiffness, and processing limitations of carbon granules. Recently, the growing demand for newer, more efficient air purification technologies has piloted research in the development of porous metal-organic frameworks (MOFs) as a promising alternative. MOFs are crystalline, microporous materials known for their tunable porosity and catalytic reactivity. However, their applications are limited due to poor environmental stability and existing primarily as free-flowing powders. This research employs the use of polymeric supports to broaden MOF applications. Polymerized high internal phase emulsions (PolyHIPEs) were used as a template to synthesize compressible, porous, composite foams with increasing amounts of embedded ZIF-8, a Zeolitic imidazolate framework, in hopes of eventually reducing the reliance on carbon filters. The foam composites were synthesized via a 90:10 water-in-oil emulsion. The internal organic oil phase was comprised of commercial hydrophobic methacrylate monomers and a surfactant while the internal aqueous phase consisted of ZIF-8 dispersed in distilled water. The aqueous phase was added dropwise to the organic phase, dispersed under high shear (500 – 1000 rpm), and polymerized overnight at 75 ℃. Scanning Electron Microscopy (SEM) and pore/throat diameter analysis confirmed that the presence of ZIF-8 enhances emulsion stability during polymerization by limiting droplet coalescence and pore collapse. Thermogravimetric analysis (TGA) revealed diminishing returns in MOF retention at higher loadings, attributed to ZIF-8 loss during purification. Microbreakthrough testing under 80% relative humidity and a 100 mg/m3 SO2 challenge feed concentration demonstrated a positive correlation between SO2 loading and increased MOF content. Furthermore, the results for the Z33 sample show an optimal balance of experimental MOF retention, emulsion stability, and SO2 absorption. This research highlights the effectiveness and versatility of emulsion-templated foams for air filtration, confirming that these systems are promising for next-level chemical filtration. Ongoing work explores in situ ZIF-8 growth, postsynthesis growth on foam surfaces, as well as the incorporation of mixed MOF systems incorporating ZIF-8 and UiO-66 to enhance multifunctionality, efficiency, and tunability. This research underscores the potential of emulsion templating and MOF-polyHIPE foam composites as high-performance, scalable alternatives to traditional carbon filters.

Poster 33
Title: Examining Local Electric Field Effects in Conducting Polymers using Vibrational Spectroelectrochemistry

Presenting Author: Ryan Spencer (Graduate Student) – Auburn University

Abstract: Conducting polymers (CPs) are central to energy storage and bioelectronic applications due to their solution processability, chemical tunability, and flexible nature. The conjugated framework of the polymer enables electronic transport, while its side chains swell with electrolyte and enable ion intercalation and transport within the polymer film. Whenever a CP is electrochemically oxidized, this creates a charge carrier on the backbone of the polymer known as a polaron, which electrostatically interacts with a counterion from the electrolyte. The polaron's conductivity is influenced by the position of the counter anion, which can impede charge transport within the polymer film due to electrostatic trapping. Furthermore, nanostructural dynamics that occur during charging of the polymer can modulate the polaron-ion interactions, which influences the trapping (localization) of the polaron. There have been a few attempts to estimate the localization of the counter anion using mid-infrared spectroscopy. However, these techniques are limited to chemical doping, and the key optical features can be spectroscopically shrouded. In this work, a carbonyl vibrational probe is introduced to the side chain of a CP to investigate the local electrostatic interactions between the polaron and counter anion. Using FTIR spectroelectrochemistry, we observed a vibrational Stark shift that responds to the encroachment of the counter anion and the trapping of polaron. The local electric field along the carbonyl bond was calculated using its Stark Tuning rate, which was determined using a combination of molecular dynamic simulations and vibrational solvatochromism experiments. The Stark Tuning rate was found to be 1.1554 cm^(-1)/(MV/cm) and the total change in electric field at the highest doping level was found to be -5.11 MV/cm. This study provides a novel way to measure the polaron and counter anion interactions by utilizing FTIR and visible/near-infrared spectroelectrochemistry

Poster 34

Title: Tracking Photodoping in a P3HT Film using Absorbance Spectrophotometry

Presenting Author: Sarah Klinger (Undergraduate Student) – Auburn University

Abstract: Doped organic mixed ionic electronic conductors (OMIECs) are conductive materials with potential applications in bioelectronics and energy storage. While electrochemical doping is typically used to boost polymer conductivity, recent work has demonstrated photoredox doping as a cheaper and more controlled alternative. In photoredox doping, a photocatalyst is optically excited to induce electron transfer with the polymer. However, this photodoping process remains poorly understood and methods for improving doping are lacking. The purpose of this experiment is to determine the factors that influence the photoredox doping of organic polymers such as poly(3-hexylthiophene), or P3HT. P3HT films were doped with 450 nm light using photocatalytic solutions containing the photocatalyst 9-mesityl-10methylacridinium tetrafluoroborate (Mes-Acr-Me+) in the electrolyteâ€¯ lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) . The extent of doping was measured by VIS-NIR absorbance spectroscopy over time, which gives insight into the electronic nature of the polaron and the rate that the polaron is created. Using this method, we investigated the impact of the photocatalyst and counterion ratio on the extent of doping. The results suggested that photodoping is strongly dependent on both the electrolytic swelling of the polymer and the electrostatic stabilization of the polaron by an ion from the electrolyte. This study demonstrates the importance of considering steric hindrance from the polymer side chains and its impact on polymer swelling for more efficient doping.

Poster 35

Title: Spectrochemical Investigation of the Break-In Effect of ProDOT (OE)-DMP

Presenting Author: Trevor Hayes (Undergraduate Student) – Auburn University

Abstract: ProDOT (OE)-DMP is a conjugated polymer useful in bioelectronic applications due to its biocompatibility and ability to conduct both ionic and electronic charge. When in use in electrochemical devices, the polymer exhibits a break-in effect, where a change in structure enables greater ionic transport resulting in enhanced conductivity. Understanding the break-in effect of the polymer allows for deeper insight into the dynamics of the doping process, which could help with the design of more consistent electronic devices. To study this break-in effect, this research uses cyclic voltammetry (CV) and absorbance spectrophotometry, which both initiate and record changes that occur during the doping process. CV was used to dope the polymer, while its voltammogram showed a drastic change in both the shape and the oxidation onset after the first cycle due to break-in. In addition, both the absorbance spectra and kinetics recorded during CV exhibited drastic changes after the first cycle, with the changes stopping after the seventh cycle. The unique changes in both the CV and kinetics indicate structural changes at the molecular level that directly impact the polymerâ€™s electrical properties.

Poster 36

Title: Computational Study of Capture and Activation of N2 Using Transitional Metal Anions

Presenting Author: Sam Lenz (Undergraduate Student) – Auburn University

Abstract: The ability to capture and activate nitrogen is essential for life on earth as it is the key component to fertilizer. Previously this could only be done through bacteria, but with the Haber-Bosch industrial process global fertilizer production was obtained. However, due to the cost and environmental concerns, other methods are being explored. Our goal is to computationally analyze the ability of the first and second row transitional metal anions to capture and activate atmospheric nitrogen without the use of ligands or catalysts. Here we present the data that while most of the metals were able to capture N2 few were able to activate it. Additionally, we present the relative energies involved and discuss how the ionization energy of the materials affects the reaction.

Poster 37
Title: Enhanced thermal and mechanical properties of Polyethylene (PE) and Polypropylene (PP) blends using self-assembling small molecules.

Presenting Author: Armin Seyed Esfahani (Graduate Student) – Auburn University

Abstract: Polyethylene (PE) and Polypropylene (PP) are among the most used plastics in the world. However, they are very difficult to sort and separate during the recycling process and often end up in a combined waste stream. Their physical properties are very similar, but they are thermodynamically incompatible, which results in products with poor properties. In this study, a self-assembly mechanism of a sorbitol derivative is used to improve thermal and mechanical properties of PE/PP blends. One of the interesting characteristics of sorbitol derivatives is that they can form a fibril network structure during the cooling process after melting. Differential scanning calorimetry (DSC) thermograms demonstrated that sorbitol derivatives disrupt the co-crystallization behavior in PE and PP blends and exhibited distinct and individual crystallization behavior in HDPE and PP blends. The DSC results further indicated that, regardless of mixing order, the incorporation of sorbitol derivatives results in an increase in the crystallization temperature of PP, showing that it acts as nucleating agents within the PP matrix and increase its crystallinity. Rheological measurements show distinct increases in complex viscosity during the cooling process that align with the DSC crystallization behavior and confirm the nucleating effect of sorbitol derivatives in PP regardless of mixing order. Moreover, mechanical measurements show that across all the samples incorporation of sorbitol derivatives improves Young's modulus and yield strength of the blends, and also samples with higher amount PP indicates higher Young's modulus and yield strength. So, both the PE/PP/sorbitol system and the PP content play important roles in enhancing the Young's modulus and yield strength.

Poster 38
Title: D2A21, a Synthetic Membrane-Interactive Peptide, Induces Cytotoxicity and Inhibits Migration in Gastric Cancer Cells

Presenting Author: Eslam Abdelazim (Graduate Student) – Tuskegee University

Abstract: Digestive tract cancers remain a major cause of cancer-related mortality in the United States and worldwide and contribute significantly to cancer health disparities in Alabama. Gastric cancer (GC) is the third leading cause of cancer mortality globally and has an approximately 33% five-year survival rate in the United States, highlighting the urgent need for novel therapeutic strategies. Lytic peptides are key components of innate immune defense that exert antimicrobial activity by disrupting microbial membranes. Emerging evidence indicates that these peptides can also selectively target tumor cells by disrupting their membranes, leading to rapid cytotoxicity. Peptidyl membrane-interactive molecules (MIMs) are synthetic lytic peptides engineered to enhance membrane-targeting antitumor activity. D2A21, an α-helical MIM peptide, has demonstrated cytotoxic effects in prostate and breast cancer cell lines. However, its potential antitumor activity in gastric cancer has not been investigated. Aim: To determine the effects of the synthetic lytic peptide D2A21 on cytotoxicity and migration in gastric cancer cells. Methods: Human gastric cancer AGS cells were treated with increasing concentrations of D2A21 (5–20 μM). Cell viability was assessed using an MTT assay following peptide treatment. Cell migration was evaluated using a wound-healing assay, and wound closure was quantified by microscopy at 24, 48, and 72 hours. Results: D2A21 treatment significantly reduced AGS cell viability in a concentration- and time-dependent manner across all time points examined. The cytotoxic effect was more pronounced at later time points, with maximal inhibition observed at 72 hours. In addition, D2A21 markedly suppressed gastric cancer cell migration, as demonstrated by a significant reduction in wound closure in the wound-healing assay. These findings indicate that D2A21 not only reduces gastric cancer cell survival but also inhibits migratory behavior associated with tumor progression and metastasis. Conclusion: The synthetic lytic peptide D2A21 induces cytotoxicity and suppresses migration in AGS gastric cancer cells, supporting the concept that membrane-targeting peptides may represent a promising therapeutic strategy for gastric cancer. Further studies are warranted to define the molecular mechanisms underlying D2A21-mediated antitumor activity and to evaluate its potential as a novel peptide-based anticancer therapy.

Poster 39

Title: Characterizing Tunnel Gating Dynamics in Soluble Methane Monooxygenase: Understanding Substrate Access in a Key Enzyme for Greenhouse Gas Mitigation

Presenting Author: Okikiola Falua (Graduate Student) – Auburn University

Abstract: Methane traps at least 28 times more heat than CO_2 over 100 years, making it a potent greenhouse gas. Remarkably, soluble methane monooxygenase (sMMO) can convert this greenhouse gas to methanol at room temperature by breaking methane's strong C-H bond (105 kcal/mol); a reaction that requires extreme temperatures, high pressures, and massive energy consumption industrially. The enzyme consists of three protein components: hydroxylase (MMOH), regulatory protein MMOB, and reductase MMOR, which work together to catalyze methane oxidation. MMOH contains a dinuclear iron cluster generating intermediate Q $((\mathrm{Fe}_2^{4+}\text{-}(\mu\text{-O})_2)$, capable of breaking this bond. A recent room temperature crystallography study revealed that MMOB opens a small-molecule tunnel called the W308- tunnel (3-4 Å wide) connecting the protein surface to the active site. While sMMO can oxidize various hydrocarbons, this tunnel provides specificity for methane. A similar tunnel prevents the overoxidation of methanol. A V41R mutation in MMOB introduces a bulky arginine residue at the tunnel entrance, physically obstructing substrate entry and thereby decreasing O_2 binding rates 25,000-fold. This appears to confirm that this tunnel is essential for O_2 and hydrocarbon substrate entry. However, crystal structures can't reveal which gates open first, how long opening takes, where bottlenecks occur, or how MMOB binding at the MMOH protein surface triggers opening of gates deep within the protein. This project aims to characterize tunnel gating dynamics in sMMO and determine how MMOB controls methane access to the active site. Molecular dynamics simulations will be performed on three systems: oxidized MMOH, reduced MMOH, and the MMOH:MMOB complex using GROMACS. Tunnel diameter fluctuations, bottlenecks, and distances between key gating residues will be analyzed using CAVER to quantify opening frequencies and coordinated gate motions. We hypothesize that the MMOH tunnel without MMOB stays closed, while MMOB-bound MMOH shows sequential gates opening events. Understanding how this enzyme efficiently captures methane could guide the engineering of biocatalysts for ambient methane oxidation and greenhouse gas mitigation.