ACS Local Section
East Alabama/West Georgia

# EAST ALABAMA/WEST GEORGIA ACS LOCAL SECTION
# 2025 ANNUAL MEETING RESEARCH SYMPOSIUM

COLUMBUS STATE
UNIVERSITY

## MARCH 1, 2025

**CORN CENTER FOR THE VISUAL ARTS**
**COLUMBUS STATE UNIVERSITY**

**ORGANIZERS**
BYRON FARNUM, CHAIR, ACS LOCAL SECTION, AUBURN UNIV
MONICA FRAZIER, COLUMBUS STATE UNIV
JONATHAN MEYERS, COLUMBUS STATE UNIV

ACS Local Section
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# East Alabama / West Georgia ACS Local Section Research Symposium

Columbus State University
Columbus, GA
March 1, 2025

**Organizers**

Jonathan Meyers – *Associate Professor – Columbus State University*

Monica Frazier – *Professor – Columbus State University*

Byron Farnum – *Associate Professor – Auburn University*

## General Schedule of Events

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|---|---|
| 9:00 am – 9:30 am | **Sign-In** – Corn Center for the Visual Arts |
| 9:30 am – 9:45 am | **Welcome Address** – The Bo Bartlett Center |
| | **(Only water or clear liquids allowed in the Gallery. No Tea, coffee, or dark colas)** |
| 10:00 am – 11:40 am | **Oral Presentation Sessions**<br>**Corn 150 –** *Inorganic Chemistry, Dr. Floyd Jackson - Moderator*<br>**Corn 176 –** *Physical Chemistry. Dr. Christopher Grieco - Moderator*<br>**Seaboard 019 –** *Analytical, Biochemistry, Materials and Organic Chemistry, Dr. Ansley Felix, Moderator* |
| 12:00 noon – 1:30 pm | **Lunch** – Bo Bartlett Center, inside Corn Center for the Visual Arts |
| 1:30 pm – 3:00 pm | **Poster Presentation Session** – Corn Center for the Visual Arts, Grand Lobby |
| 3:30 pm – 4:00 pm | **Awards Ceremony/Closing Remarks –** The Bo Bartlett Center<br>Dr. Byron Farnum – *Associate Professor – Auburn University*<br>Chair, ACS Local Section |

All times are Eastern Standard Time

## Oral Presentations – Corn 150
## Inorganic

Moderator: Dr. Floyd Jackson

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|---|---|---|
| 10:00 am | *Mechanism guided two-electron energy storage for redox-flow batteries using nickel bis(diphosphine) complexes* | **Md Musharraf Hossain**<br>Graduate Student<br>Auburn University |
| 10:20 am | *Molecular Co(II) electrocatalysts with quinol tethered ligands for homogeneous electrocatalytic oxygen reduction reaction (ORR)* | **Maksuda Parvin**<br>Graduate Student<br>Auburn University |
| 10:40 am | **Break** | |
| 11:00 am | *Tuning polar E-H bond activation with a cobalt(II) complex bearing a non-trigonal phosphorus center* | **Pamodya Weerasuriya**<br>Graduate Student<br>Auburn University |
| 11:20 am | *Redox-Active Quinol Ligand Complexes as Highly Efficient Catalase Mimetics: Expanding Antioxidant Strategies with Mn(II), Fe(II), and Zn(II)* | **Sana Karbalaei**<br>Faculty<br>Tuskegee University |

All times are Eastern Standard Time

# Oral Presentations – Corn 176
## Physical

Moderator: Dr. Christopher Grieco

| | | |
|---|---|---|
| 10:00 am | *Use of Fluorescence Probe Spectroscopy to Characterize RH-Dependent Phase Transitions and Other Physicochemical Properties of Respiratory Aerosols* | **Angel Gibbons**<br>Graduate Student<br>Auburn University |
| 10:20 am | *Zinc enhanced 2e- redox chemistry for Ni(IV/II) diethyldithiocarbamate couple* | **Smriti Somai**<br>Graduate Student<br>Auburn University |
| 10:40 am | **Break** | |
| 11:00 am | *Utilizing Vibrational Probes to Study the Polaron-Anion Induced Electric Field in a Conducting Polymer* | **Ryan Spencer**<br>Graduate Student<br>Auburn University |
| 11:20 am | *In situ monitoring of charge carriers in PEDOT:PSS using spectroelectrochemistry* | **Caitlyn Clark**<br>Graduate Student<br>Auburn University |

All times are Eastern Standard Time

# Oral Presentations – Seaboard 019
## Analytical, Biochemistry, Materials, and Organic

Moderator: Dr. Ansley Felix

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|---|---|---|
| 10:00 am | *Optimization of the Performance of DNA Monolayer-based Electrochemical Sensors Through the Study of Surface Properties.* | **Mainul Mazumder**<br>Graduate Student<br>Auburn University |
| 10:20 am | *Synthesis of bis[Cyclic(alkyl)(amino)Carbenes] for Methane to Methanol Conversion* | **Chase Ledbetter**<br>Graduate Student<br>Auburn University |
| 10:40 am | **Break** | |
| 11:00 am | *Hemp hurd: A biomass for creating sustainable composite materials* | **Arun Ghosh**<br>Faculty<br>Troy University |
| 11:20 am | *A study on the commercial beverages to suppress the reactive oxygen species produced by ultrasound in water* | **Duk (Daniel) Kim**<br>Faculty<br>Auburn University - Montgomery |

All times are Eastern Standard Time

# Oral Presentations (alphabetical) – Corn Center for the Visual Arts

## Clark, Caitlyn – Graduate Student, Auburn University

**Authors:** Caitlyn Clark
**Title:** In situ monitoring of charge carriers in PEDOT:PSS using spectroelectrochemistry

**Abstract:** Organic mixed ionic-electronic conductors (OMIECs) emerge as promising materials for enhancing flexible bioelectronics due to their dual capability to conduct both ionic and electronic charges. Conjugated polymers (CPs), a distinct subclass of OMIECs, can transition between semiconducting and conducting states through electrochemical doping, which adds or removes charge carriers along the ð�œ‹-conjugated polymer backbone. However, the structural and morphological changes that occur during doping can unpredictably affect the performance of electrochemical devices. Therefore, additional in situ methods are needed to investigate these changes and develop design principles for high-performance OMIEC devices. In this work, we introduce an ultrafast pump-probe spectroelectrochemistry (SEC) method for detecting charge carriers in a model depletion mode CP system, Poly(3,4 ethylenedioxythiophene) :poly(styrenesulfonate)(PEDOT:PSS).We show that the spectral signatures of the polaronic, bipolaronic, and neutral states of PEDOT:PSS in the visible and near-infrared (400-2300 nm) can be observed and tracked as a function of device bias. Voltage-dependent excited state dynamics of the charge carriers reveal new insights into their behaviors during mixed ionic-electronic conduction.

## Ghosh, Arun – Faculty, Troy University

**Authors:** Arun Ghosh
**Title:** Hemp hurd: A biomass for creating sustainable composite materials

**Abstract:** Hemp hurd is a lignocellulosic biomass derived from the stem of natural hemp fiber. It was processed using a high-shear thermo-mechanical method in combination with recycled polypropylene/polyethylene (PPE) at a 50/50 mass ratio to create sustainable composite materials with enhanced mechanical performance and improved melt-flow behavior. Various characteristics were analyzed, including tensile stress-strain, dynamic mechanical viscoelasticity, melt rheology, X-ray diffraction, and scanning electron microscopy (SEM) images. In the composite, PPE was partially replaced with polypropylene-graft-maleic anhydride (PPgMA) to improve interfacial adhesion and mechanical performance. The neat material, composed of 50/50 blends of hemp hurd and PPE, exhibited an average tensile strength of 11.4 MPa and a Youngâ€™s modulus of 2.8 GPa. When a portion of the PPE phase was replaced with PPgMA, significant improvements in both tensile strength and stiffness were observed. Notably, the blend consisting of hemp hurd, PPE, and PPgMA in a ratio of 50/45/5 showed remarkable mechanical performance, with an average tensile strength of 26.5 MPa and a Youngâ€™s modulus of 3.2 GPa. The melt rheology analysis indicated that the materials' storage modulus and complex viscosity were frequency-dependent. As the angular frequency increased, the viscosity decreased while the modulus increased, suggesting that the composites behave like traditional thermoplastics. SEM imaging demonstrated that PPgMA enhanced interfacial adhesion within the blend, which correlated with  improvements in tensile strength, modulus, and melt viscosity. In summary, bio-renewable hemp hurd has the potential to produce materials with enhanced mechanical performance and good thermal recyclability for a variety of technical applications.

## Gibbons, Angel – Graduate Student, Auburn University

**Authors:** Angel M. Gibbons, Paul E. Ohno

**Title:** Use of Fluorescence Probe Spectroscopy to Characterize RH-Dependent Phase Transitions and Other Physicochemical Properties of Respiratory Aerosols

**Abstract:** Understanding the viability of viruses contained in respiratory particles and the connections between this viability and the relative humidity (RH)- mediated physicochemical properties of the particles themselves is critical to mitigate respiratory disease transmission. Here we present the use of fluorescence probe spectroscopy to investigate the phase state of model respiratory particles. In this technique, fluorescent molecules are incorporated into the particles of interest and their polarity-dependent emission properties are used to determine particle phase state. Particles consisting of mucin/salt mixtures, a growth medium, and simulated lung fluid were studied across an RH range of 30-80%. Phase separation between the organic and inorganic constituents was observed at an RH that was dependent on the chemical composition of the particles. Furthermore, we demonstrate that volatilization of probe molecules and subsequent condensation can be used to incorporate the molecules into preexisting particles. This technique will enable the study of real exhaled respiratory particles using fluorescence probe spectroscopy. Finally, we discuss preliminary results using fluorescence probe spectroscopy to investigate other physicochemical properties such as pH and viscosity.

## Hossain, Md Musharraf – Graduate Student, Auburn University

**Authors:** Md Musharraf Hossain, Byron H. Farnum

**Title:** Mechanism guided two-electron energy storage for redox-flow batteries using nickel bis(diphosphine) complexes

**Abstract:** The unique architecture of redox flow batteries (RFBs), which decouples 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 (Î”G = -nFEcell) depends on the number of electrons (n) transferred per molecule and the potential difference between catholyte potential (Ec) and anolyte potential (Ea) where Ecell = Ec - Ea. Increasing energy density and finding redox-active molecules of high stability are the two main challenges for practical use of RFBs. In this study, we investigated easily synthesized, highly stable, and soluble nickel(II) bis(diphosphine) complexes for anolytes in RFBs, which undergo electrochemically reversible two-electron redox reactions at notably negative reduction potentials in acetonitrile (MeCN) solvent. For example, [Ni(dmpe)2](BF4)2, where dmpe = 1,2-bis(dimethylphosphino)ethane, undergoes a reversible 1 x 2e-reduction to Ni(dmpe)2 at -1.36 V vs Fc+/0 and exhibits solubility about 1 M in MeCN. Our studies have shown that halide (X- = Cl, Br, I) electrolyte conditions have significant impact on solubility, electrochemistry, and cycling stability of nickel(II) bis(diphosphine) complexes. It has been observed that the Xâ» ions increase the reduction potential to a more negative value, convert 2 x 1e- redox process to 1 x 2e- redox reaction, and enhance the charge-discharge cycling performance. We also found that addition of diphosphine ligands further improve the cycling performance of nickel(II) bis(diphosphine) complexes. Our focus will be the comprehensive understanding of redox mechanism of nickel (II) bis(diphosphine) complexes by analyzing data from scan rate dependent cyclic voltammetry (CV) studies, DigiElch modeling, UV-vis spectroscopy, and 31P NMR spectroscopy. The insights gained from this research will enhance our understanding of using multi-electron inorganic redox couples and design new complexes as suitable anolytes for practical RFB applications.

### Karbalaei, Sana – Faculty, Tuskegee University

**Authors:** Sana Karbalaei, Ivana IvanoviÄ, BurmazoviÄ, and Christian R. Goldsmith
**Title:** Redox-Active Quinol Ligand Complexes as Highly Efficient Catalase Mimetics: Expanding Antioxidant Strategies with Mn(II), Fe(II), and Zn(II)

**Abstract:** Reactive oxygen species (ROS), such as hydrogen peroxide ($H_2O_2$) and superoxide ($O_2$), play significant roles in oxidative stress, contributing to various health conditions. While superoxide dismutase (SOD) mimetics have been widely explored, the development of efficient catalase mimics remains challenging. In our previous work, we demonstrated that quinol-containing ligands enable manganese complexes to mimic SOD activity, and even Zn(II) complexes can facilitate superoxide degradation through ligand-based redox chemistry. Expanding on this approach, we investigated the catalytic activity of Mn(II), Fe(II), and Zn(II) complexes with 1,8-bis(2,5-dihydroxybenzyl)-1,4,8,11-tetraazacyclotetradecane (Hâ‚„qpâ‚„), a macrocyclic quinol-based ligand, to determine their ability to degrade $H_2O_2$. While only the Mn(II) complex displayed measurable SOD activity, all three metal complexes exhibited exceptionally high catalase-like activity. Notably, the Zn(II) complex catalyzed $H_2O_2$, decomposition, marking the first known instance of a redox-inactive metal complex successfully catalyzing ROS degradation. These findings highlight the potential of ligand-centered redox chemistry in designing antioxidant mimetics and offer new directions for developing therapeutic agents targeting oxidative stress-related diseases.

### Kim, Duk (Daniel) – Faculty, Auburn University Montgomery

**Authors:** Chanju Chung, Alexandra Jackson, and Duk Kyung Kim
**Title:** A study on the commercial beverages to suppress the reactive oxygen species produced by ultrasound in water

**Abstract:** It has been reported that the increased level of ROS leads to oxidative stress and disease. The body has antioxidant defense, and a positive health effect from consuming healthy beverages with high antioxidant capacity may be expected to lower the level of risks in chronic diseases. Ingredients in beverages are eventually infused in the body fluid where various forms of reactive oxygen species (ROS) are produced endogenously by mitochondria and NADPH oxidases. Artificial ROS in this study was produced by ultrasonic irradiation to the beverage-mixed water. A fluorometric method was applied to measure the amounts of peroxides to measure the suppression level. Various beverages solutions were tested including fruit-originated juices, brewed beverages, alcoholic beverages, and popular sodas. The general trend of ROS suppression from wine or fruit juice shows a rough trend of more antioxidizing with the darkness of the wine or juice. Green tea is a lightly colored antioxidant beverage more effective than processed teas, which are darker in color. The addition of well-known antioxidant Vitamin C makes every fruit juice effectively anti-oxidizing.

## Ledbetter, Chase – Graduate Student, Auburn University

**Authors:** Chase Ledbetter

**Title:** Synthesis of bis[Cyclic(alkyl)(amino)Carbenes] for Methane to Methanol Conversion

**Abstract:** Methane, known for its potent heat-trapping capabilities as a greenhouse gas, presents significant environmental challenges. Converting methane into valuable chemicals such as methanol is essential, given methanol's broad applications in pharmaceuticals, resins, and dyes. However, this conversion is hindered by the substantial energy required to break carbon-hydrogen bonds without over oxidation of methane to other byproducts like formaldehyde. Recent computational studies have suggested using low valent metal-oxo complexes may be the key to this conversion. This work explores an innovative approach centered on the use of cyclic (alkyl)(amino)carbenes (CAACs), neutral L-type ligands with promising potential to stabilize electron-rich low-oxidation state transition metals. Most examples of CAACs used in catalysis involve the use of one or two CAAC ligands coordinating to a metal center. However, this work focuses on the synthesis of a bisCAAC ligands involving two CAACs that are tethered together using an aryl-backbone. The electronic properties of the carbenes and the pyridyl-backbone may enhance the ability for the ligand to chelate to a metal center. With the only reported example of a low-valent metal-oxo complex involving rhenium (0), efforts are being made toward using these bisCAACs to stabilize electron rich metal-oxo complexes involving both rhenium and iron. The synthesis of a low valent iron-oxo complex could be lucrative due to their usage in sMMO enzyme biological systems.

## Mazumder, Mainul – Graduate Student, Auburn University

**Authors:** Mainul Islam Mazumder, Asanka Gurukandure, and Christopher J. Easley*

**Title:** Improving DNA Monolayer-based Electrochemical Sensors through Engineering the Temporal Response

**Abstract:** DNA monolayer-based electrochemical sensors have gained attention recently due to high sensitivity, specificity, and fast label-free detection. Ease of miniaturization and real-time monitoring capabilities make these sensors a potential candidate for point-of-care diagnosis. Previously, our research group reported a DNA-based electrochemical bowtie sensor where a thiolated DNA (thio-DNA), analyte-conjugated DNA, and methylene blue (MB) tagged DNA (MB-DNA) were ligated on a 2D gold-on-glass electrode. Antibody binding to the sensor slows down the tethered diffusion of MB molecules and eventually reduces the electrochemical signal upon square wave voltammetry (SWV) interrogation. Higher SWV frequency gives a high faradaic current yet with high non-faradaic current interference. On the other hand, faradaic and non-faradaic current in surface-confined systems decays with time, and the signal-to-noise ratio is very low at low frequencies. In this study, we modified the MB-DNA of our bowtie sensor to get significantly high faradaic current even at low SWV frequencies. Moreover, the tethered diffusion of the MB molecules was tuned by adding spacers of different lengths (4-12 nucleotides) and flexibilities (varying polyethylene glycol (PEG) lengths) to the thio-DNA. The goal is to slow down the decay of faradaic current and enable the harvesting of significant faradaic current with negligible non-faradaic interference at low SWV frequencies. As a proof of concept, we utilize the hybridization of MB-DNA and complementary thio-DNA. The modified MB labels exhibited higher faradaic currents compared to the unmodified labels. Moreover, the increase in spacer length increased the faradaic current at low SWV frequencies, likely because it takes a longer average time for the MB molecules to reach the surface to transfer electrons. When the modified MB label was kept furthest away (12 nucleotides) from the surface, we observed sufficient faradaic current (252 nA) with negligible non-faradaic contribution (~3 nA) at 10 Hz. However, PEG spacers exhibit comparatively low current at low SWV frequencies, as the tethered diffusion is faster. This issue is advantageous for bowtie sensors, where after antibody binding, a significant faradaic current could still be observed at 3-10 Hz when the modified MB-DNA is furthest away from the surface and using PEG spacers. These results suggest that chronoamperometry with delayed sampling time can replace SWV to interrogate the electrode. A custom-built potentiostat could be a cheaper alternative with engineered temporal responsiveness for these sensors. Moreover, the modified MB-DNA can be utilized to improve the sensitivity of different other DNA monolayer-based sensors.

## Parvin, Maksuda – Graduate Student, Auburn University

**Authors:** Maksuda Parvin, Segun V. Obisesan, Christian R. Goldsmith, and Byron Farnum

**Title:** Molecular Co(II) electrocatalysts with quinol tethered ligands for homogeneous electrocatalytic oxygen reduction reaction (ORR)

**Abstract:** Global energy demand and environmental concerns require substituting nonrenewable fossil fuels with low-cost, environmentally friendly, sustainable energy systems. Promising alternatives in this respect are fuel cells and metal ion batteries. However, the cost and reliability of the catalysts used in fuel cells pose significant barriers to commercialization. An ideal electrocatalyst should be selective for reducing O2 to H2O rather than H2O2, highly active, capable of operating at a low effective overpotential, stable in the acidic media required for ORR catalysis, and readily synthesizable from inexpensive starting materials. Oxygen reduction is carried out in living organisms by enzymes such as cytochrome c oxidase (CcO) that utilizes transition metals. The abundance and accessibility of first-row transition metals, the characterization of active sites, the fundamental understanding of catalytic steps, and synthetic modifications for mechanistic hypotheses inspired the development of homogenous molecular catalysts. Incorporating one or more redox-active quinols in ligand structures of the electrocatalyst has successfully promoted ORR and improved product selectivity. Prior research from our lab showed that incorporating quinol moiety on ligand scaffold, a Co(II) complex selectively produces H2O from O2 at a low overpotential.

Recently, complexes of Fe(II) and Fe(III) complexes with quinolic ligands have been found to serve as effective electrocatalysts. We have prepared Co(II) complexes with N-(2,5-dihydroxy benzyl)-N,N-bis(2-phenylmethyl)-1,2-ethylenediamine (H2qp3) and N,N-bis(2,5-dihydroxy benzyl)-N,N-bis(2-phenylmethyl)-1,2-ethylenediamine (H4qp2). We investigated their ability to serve as electrocatalysts for ORR as well as acid/base reactivity. The complex with two quinols in the ligand scaffold (i.e., Co(H4qp2)2+) enhances catalytic activity compared to the catalyst with a single quinol (i.e., Co(H2qp3)2+) at the cost of higher overpotential.

## Somai, Smriti – Graduate Student, Auburn University

**Authors:** Smriti Somai, Belinda Allotey, and Byron Farnum
**Title:** Zinc enhanced 2e- redox chemistry for Ni(IV/II) diethyldithiocarbamate couple

**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, currently RFBs have a lower energy density than LIBs. Multi-electron redox chemistry of molecules at a single potential have been shown to increase energy density. Nickel(II) N,N-diethyldithiocarbamate (Ni(II)(dtc)2) undergoes 2e- ligand coupled electron transfer to form [Ni(IV)(dtc)3]+ upon oxidation and goes back to Ni(II)(dtc)2 when reduced. CV experiments in MeCN and TBAPF6 show 1 two-electron oxidation wave while the reduction displays 2 sequential one-electron 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. Addition of zinc salts causes the sequential one-electron reduction waves to combine into 1 two-electron reduction wave changing the mechanism to ECE where the chemical step is catalyzed by zinc. The zinc salts used in this study are: Zn(ClO4)2, Zn(BF4)2, ZnCl2, Zn(NO3)2 and Zn(OTf)2. Additionally, when Zn(II)dtc2 is added to Ni(II)(dtc)2, an increase in current on the oxidation side is observed while having the same effect as previously mentioned on reduction side. This occurs because Zn(II)dtc2 delivers the additional ligand needed to form [Ni(IV)(dtc)3]+ during oxidation. During reduction it removes the additional ligand to form Ni(II)(dtc)2. While Zn salts certainly enhance the two-electron behavior, there are differences in the rate of the chemical step due to the coordination geometry around the Zn(II) ion. CV and SWV were used to study the electrochemical mechanisms. NMR and UV/Vis spectroscopy were used to study the binding of zinc salts to the nickel complex. ZnCl2 was found to have the lowest binding to Ni(II)(dtc)2 because of the strongly coordinating Cl- ions.

## Spencer, Ryan – Graduate Student, Auburn University

**Authors:** Ryan Spencer, Caitlyn Clark, and Christopher Grieco
**Title:** Utilizing Vibrational Probes to Study the Polaron-Anion Induced Electric Field in a Conducting Polymer

**Abstract:** Conducting Polymers (CPs) are central to energy storage and bioelectronic applications due to their solution processability, chemical tunability, and variable conductivity. The conjugated frame in the backbone of the CPs enables electron transport throughout the entire structure. The side chains of the enable the polymer to swell with electrolytes to intersperse counter anions into the polymer. Whenever a CP is oxidized, this creates a charge carrier on the backbone of the polymer known as a polaron. After doping, the polaron and the counter anion create an electrostatic field, and the interactions between them affect the polaron's conductivity. Current techniques, such as steady state absorbance, ultrafast spectroscopy, and electrochemistry, are unable to precisely study these interactions. In this work, a carbonyl vibrational probe was introduced to the side-chains of a model CP to investigate the electrostatic interactions between the polaron and counter anion. Using FTIR spectroscopy, we observed a vibrational Stark shift that depends on the doping level of the CP. This indicates that the carbonyl is able to sense the change in the electric field. Our results demonstrate a new way to study the polaron using FTIR spectroscopy, which leverages the sensitivity of vibrational probes.

## Weerasuriya, Pamodya – Graduate Student, Auburn University

**Authors:** Pamodya Weerasuriya, and Ethan Hill

**Title:** Tuning polar E-H bond activation with a cobalt(II) complex bearing a non-trigonal phosphorus center Polymer

**Abstract:** Second-row transition metals have been the preferred choice for activating polar E-H bonds (O-H, S-H, B-H and N-H). However, their scarcity and high cost have driven interest in more economical alternatives. A promising strategy involves employing first-row transition metals alongside metal-ligand cooperativity. While E-H bond activation typically follows a two-electron mechanism, first-row metals often exhibit a preference for single electron pathways. Nevertheless, with strategic ligand design, these metals can be tuned to facilitate two-electron processes. This study explores the synthesis of a cobalt(II) complex featuring a non-trigonal phosphorus center. Non-trigonal phosphorus compounds are known to independently activate E-H bonds due to their ambiphilic nature. Our goal was to determine whether a non-trigonal phosphorus ligand, when coordinated to a first-row metal, could cooperatively activate polar bonds. We present the synthesis and characterization of a novel cobalt(II) complex, K[Co(3Nurea)(OAc)], which incorporates a urea-based ligand bearing a non-trigonal phosphorus center directly bound to cobalt. Comprehensive spectroscopic analysis provides insight into its structural features, while its reactivity towards polar bonds such as B-H, Si-H, and O-H is investigated. Additionally, we examine its potential for transferring the E-H moiety to unsaturated substrates. By integrating non-trigonal phosphorus chemistry with metal-ligand cooperativity, this work offers new opportunities for catalyst development targeting the activation of challenging substrates.

# Poster Presentations (alphabetical) – Corn Center Grand Lobby

## Androutsopoulos, Alexandros – Graduate Student, Auburn University

**Authors:** Alexandros Androutsopoulos and Evangelos Miliordos

**Title:** An Insight into the Electronic Structure of (V-CO2)- Species

**Abstract:** It is well known that global warming constitutes a hard nut to crack since human activities have provoked the accumulation of greenhouse gases in the atmosphere and by extension, the increase of Earth's average surface temperature. Carbon dioxide lies among the gases in question, as the exploitation of Earth's fossil fuels has resulted in an increase of its atmospheric concentration. To mitigate this issue, scientists have examined the carbon capture and utilization (CCU) approach according to which carbon dioxide can be converted into high-value chemicals such as methane, methanol, and formic acid [1]. Methanol production is of considerable interest since it can be used as fuel, produce H2 via reforming, and serve as energy carrier [2]. As highlighted in our recent work, the use of molecular catalysts with electron rich metals (CERMAs) can be applied for the capture and conversion of CO2 into CH3OH [3]. Within this context, the present work focuses on the investigation of the interaction between vanadium anion and carbon dioxide via high-level multi-reference methods with a view to providing an accurate description of the interaction in question. To the best of our knowledge, such a fundamental theoretical study is missing from literature.

## Daramola, Charles – Graduate Student, Auburn University

**Authors:** Charles B. Daramola and Byron H. Farnum

**Title:** A Manganese Complex with a Fluxional Bipyridine Backbone Ligand for Multi-Electron Energy Storage in RFBs

**Abstract:**The critical need for highly stable and efficient redox active organometallic compounds for energy storage is increasing, particularly for redox flow batteries (RFBs), which store excess energy from renewable sources such as solar and wind. This research focuses on first-row coordination compounds. The manganese bipyridine complex featuring a benzylic diethylamine group strategically positioned in the secondary coordination sphere acts as a fluxional ligand investigated for its structural adaptability during redox cycling. This complex transitions through intermediate oxidation states, from Mn+I to Mn-I, leveraging disproportionation to allow a robust 2e- redox couple governed by metal-ligand bond formation as observed by cyclic voltammetry. This 2e- redox cycle offers a promising pathway for optimizing energy storage systems.

## Evdokimov, Andrei – Graduate Student, Auburn University

**Authors:** Andrei Evdokimov and Evangelos Miliordos

**Title:** Computational Study of Carbonyl and Aziridine Copolymerization Catalytic Reactions

**Abstract:** This study computationally investigates the various possible reaction pathways for the copolymerization of aziridine and carbonyl compounds using CH3C(O)Co(CO)4 as a precatalyst. Two pathways were found to be dominant from a kinetic perspective. One, previously described by Darensbourg et al. using in situ infrared spectroscopy, involves aziridine insertion into the cobalt-acyl bond, followed by ring opening via cobaltate anion attack and subsequent carbonyl insertion. We propose and analyze an alternative, competitive mechanism involving electron transfer from the catalyst to the substrate, followed by radical polymerization. These two pathways exhibit similar free energy barriers for their rate-limiting steps. Our computational findings indicate that solvent choice significantly influences the relative favorability of each pathway.

## Gregory, Taylor – Graduate Student, Auburn University

**Authors:** Taylor Gregory and Evangelos Miliordos

**Title:** Quantum Chemical Interpretation of Experimentally Recorded Photoelectron Spectra of Uranyl Complexes

**Abstract:** In this work, we perform high-level electronic structural calculations to examine the ground state and low-lying excited electronic states of UO2(CH3CO2)2,3 complexes. Our calculations include static, dynamic, and spin-orbit effects. The results are used to interpret and assign the peaks of these systemsâ€™ photoelectron spectrum.

## Haq, Humaira – Graduate Student, Auburn University

**Authors:** Humaira Haq, Ethan Hill*

**Title:** Effect of Oriented External Electric fields in catalysis using immobilized Metalloporphyrins

**Abstract:** In modern inorganic catalysis, researchers have shifted focus towards new means of controlling reactivity at a transition metal center. One such area involves the study of how chemical reactions can be controlled using oriented external electric fields (OEEFs). An OEEF can serve to alter reactivity by several mechanisms including controlling the orientation of substrate molecules, polarizing diffuse electron density of the substrate or metal center, or enhancing bond activation when oriented along the bond-forming or -breaking axis. The net result of these alterations by an OEEF are modulation of equilibrium constants and activation barriers. The research presented will explore the influence of OEEFs in inorganic catalysis using transition metal complexes immobilized onto a conductive surface. Self-assembled monolayers (SAMs) using a diisocyanide linker [CN-(CH2)6-NC] have been prepared. The diisocyanide serves both to bind a Ru(TPP)CO complex (where TPP = meso-tetraphenylporphyrinato) and to tether the complex at a controllable distance and orientation on conductive surfaces like gold

and fluorine-doped tin oxide (FTO). The SAM and presence of the ruthenium metalloporphyrin have been confirmed by both electrochemical (EIS, cyclic voltammetry, and linear sweep voltammetry) and spectroscopic techniques (UV-vis and sum frequency generation). The interfacial spectroscopic techniques, vibrational sum frequency generation (vSFG) is an interface-specific technique that has been used to characterize the modified electrodes using the C-N stretching frequency as a vibrational probe. Our aim is to examine how OEEF s alter reactivity at the Ru center with attention on two reaction types: ligand exchange and non-Faradayic catalysis. Firstly, ligand exchange studies using triphenylphosphine have been performed using cyclic voltammetry (CV) experiments to monitor shifts in the Ru(II)/(III) redox couple. Secondly, the non-Faradayic deformylation of organic aldehydes has been explored. We have observed that applying a +150 mV bias enhances the product yield and applying a negative voltage of -100 mV inhibits the formation of product indicating the influence of applied electric field on reactivity. The preliminary results and conclusions from these studies will be discussed. This research focuses on understanding the influence of electric fields on inorganic catalysis which will help develop new catalytic systems that harness the versatility of electric field catalysis.

## Howell, Joshua – Graduate Student, Auburn University

**Authors:** Joshua G. Howell, Joanne Y. R. Seow, & Christopher J. Easley.
**Title:** Raised Tube Architecture for Increased Normally-Closed Valve State Biasing

**Abstract:** In microfluidic devices, active fluid control relies on two valve types: normally open (NO) and normally closed (NC). NC valves work by using vacuum to bridge a gap between inlet and outlet in the working layer. The vacuum must generate enough pressure differential to overcome the adhesion between the polydimethylsiloxane (PDMS) membrane and the working layer discontinuity. Our research uses 3D-printed pneumatic components with thin (250 micrometer) PDMS membranes. Due to PDMS's low spring force, the valve opens rapidly once sufficient vacuum is applied, since adhesion rather than elasticity is the main barrier to opening. However, this same low spring force leads to slow closing times, creating a limitation for device operations like pump cycling, droplet manipulation, and logic functions. The valve design can also allow the PDMS to stick to the upper displacement chamber, requiring near-atmospheric pressure to close-- further slowing operation.

To address these limitations, we developed methods to pre-bias the PDMS membrane by modifying the working-side valve architecture. Using resin-based 3D printing enabled rapid prototyping and precise control over valve geometry. Our key innovation was adding raised margins around the inlets and outlets of the channels in the working layer, which result in significant increases (100%+) in closing pressure differentials and reduced hysteresis while still being controllable by the same house vacuum that runs all other devices in the lab. Future work will incorporate this design into existing pneumatic oscillators and pumps for direct performance comparison with traditional valves. We anticipate that the implementation of similar 3D-printed valve architectures could significantly extend the utility of NC valves across both pneumatic and microfluidic applications.

## Kanyairita, Getrude – Graduate Student, Tuskegee University

**Authors:** Getrude Kanyairita, Willard Collier and Desmond Mortley
**Title:** Industrial Hemp Extract: An Emerging Potential Source of Biopesticide

**Abstract:** Pests and diseases have caused significant problems since the domestication of crops, resulting in economic loss and hunger. To overcome these problems, copper-based bactericides are used to inhibit the proliferation of these pathogens, but resistant strains now exist. Additionally, because copper does not biodegrade, its extended use leads to accumulation in the soil which can be toxic to soil microorganisms and plants, diminishing biological activities, and causing soil infertility. The utilization of noncopper-based synthetic pesticides in plant bacteria control is not conducive to sustainable agriculture because of their adverse effects on the environment including water pollution leading to the death of aquatic organisms, soil contamination causing a decline in beneficial soil microorganisms, and the loss of beneficial insects and public health, such as cardiovascular disease, negative effects on the male reproductive system, carcinogenicity, and adverse effects on the human nervous system. There is an urgent need to develop safer and more sustainable pesticides. Plants are reservoirs of compounds that could potentially replace synthetic bactericides, fungicides, and insecticides. Numerous studies have been conducted on industrial hemp to determine the efficacy of hemp compounds against pathogens that affect humans, however, there is a knowledge gap regarding their effectiveness against plant pathogens. We determined the efficacy of industrial hemp extracts against Pseudomonas syringae pv tabaci and Erwinia carotovora bacteria which cause significant crop loss in potatoes, leaf vegetables, tobacco, coffee, papaya, and soybeans among many others. Hemp inflorescences were extracted using organic solvents and characterized using high-performance liquid chromatography/gas chromatography-mass spectrometry. The extract contained reasonably high concentrations of eight terpenes: alpha-bisabolol, alpha-caryophyllene, beta-bisabolene, beta-caryophyllene, d-limonene, nerolidol 1, nerolidol 2, and nerol acetate (0.05-0.6 mg/ml) plus cannabidiol (0.69%) all of which have antimicrobial properties. An efficacy test was conducted in vitro using different concentrations of crude extracts and revealed a minimum inhibitory concentration of 2.05 mg/ml and a non-inhibitory concentration of 1.2 mg/ml. The results indicate that Pseudomonas syringae pv tabaci and Erwinia carotovora are susceptible to hemp extracts, therefore hemp extract is a potential source of sustainable and safe biopesticides to protect the environment and human health.

## Kollaram, Apoorva – Undergraduate Student, Columbus State University

**Authors:** Apoorva Kollaram, Chayce Schuler, Gabriela Mieles
**Title:** Purification of Recombinant GFP – Preptin Fusion Proteins

**Abstract:** Preptin is a 34-residue peptide hormone, extracted from secretory granules of pancreatic ÃŸ cells. It has demonstrated promise as a therapy for two common diseases: osteoporosis and diabetes. The study aims to delve deeper into the metabolic pathway of preptin. The secondary structure and metabolic mechanism of preptin remain unknown. To begin to understand the metabolic capabilities of preptin, we are pursuing a structure-activity relationship (SAR) study of the peptide via alanine scanning mutagenesis. The following preptin residues were all singly mutated to alanine and analogs were expressed as green fluorescent fusion proteins in E. coli: P17A, V18A, G19A, W27A, R28A, Q29A. Currently, we are optimizing purification of the fusion protein in preparation of site-specific cleavage and isolation of the mutated analogs. By studying the effects of these mutations, we aim to determine which amino acids in preptin’s primary structure are vital to its metabolic activity.

## Martz, Luke – Graduate Student, Auburn University

**Authors:** Luke A. Martz and Steven O. Mansoorabadi

**Title:** Computational Investigations of Nitrogenase Homolog CfbCD Reveal Insights to its First and Last Catalytic Steps

**Abstract:** Methyl coenzyme-M reductase (MCR), the enzyme responsible for the terminal step of methanogenesis, requires a host of accessory proteins for its maturation and assembly.1 Prior work in the Mansoorabadi laboratory identified the gene cluster responsible for the biosynthesis of MCR Ni-containing cofactor F430, denoted cfb. One protein complex encoded in this cluster, CfbCD, catalyzes the unprecedented ATP-dependent addition of 6 electrons and 7 protons to Ni-sirohydrochlorin a,c-diamide (Ni-s-acd) and the cyclization of its c-acetamide side chain to a Î³-lactam ring to form 15,173-seco-F430-173-acid (seco).2-3 CfbCD itself is a member of the nitrogenase superfamily, consisting of a dimer of Fe protein homolog CfbC and a dimer of MoFe protein homolog CfbD. Both CfbC and CfbD dimers possess intersubunit [4Fe-4S] clusters. It is not yet clear if the CfbCD heterotetrameric complex itself dimerizes to form a heterooctamer analogous to common nitrogenase enzymes.4 While seco is the final characterized product of CfbCD catalysis, UV-visible absorption spectra indicate that an uncharacterized intermediate, dubbed pre-seco, forms first and slowly converts to seco over the course of ~22 h.3. In this ongoing study, we have performed constant-pH accelerated molecular dynamics (CpHaMD; performed using the Amber molecular dynamics package5) on an AlphaFold6-predicted heterotetramer model of CfbCD from Methanosarcina thermophila docked with Ni-s-acd and proposed reaction intermediate candidates (identified by comparative density functional theory (DFT) calculations using ORCA7). Preliminary data demonstrates conformational asymmetry in the CfbD2 subunit of substrate-free CfbCD. Single-substrate simulations identified a putative active site that resides primarily in only one of the CfbD monomers, while double-substrate simulations reveal the ability of Ni-s-acd to bind at two active sites in an asymmetric manner suggestive of catalytic cooperativity between the active sites. Additionally, the highly conserved residues His345 and Arg325 of CfbD maintain close contact to C17 and C18 of Ni-s-acd, respectively. This coincides with the comparative DFT studies that suggest reduction of the C17=C18 bond is the most facile. Additionally, we have performed time-dependent DFT calculations using Gaussian8 on a series of conformers obtained from molecular dynamics simulations of seco in explicit solvent to improve the accuracy of UV-visible absorption spectral predictions. Using this method we have predicted a spectrum that closely reproduces the experimentally observed spectrum of seco. Work is underway to apply this methodology to models of pre-seco candidates to gain insight into the structure of the immediate product of the CfbCD reaction.

## Nwankpa, Ugonna – Graduate Student, Auburn University

**Authors:** Ugonna D. Nwankpa, Mohtadin Z. Hashemi, Mainul I. Mazumder, Christopher J. Easley*
**Title:** Optimization of the Performance of DNA Monolayer-based Electrochemical Sensors Through the Study of Surface Properties

**Abstract:** Biosensors have revolutionized medical diagnostics in terms of reduction in cost and turn-around-time, improving sensitivity in the quantification of analytes of medical importance and increasing the feasibility of point-of-care testing. Due to their specific complementary interactions and ease of manipulation, DNA has been extensively employed in biosensor fabrication. In general, DNA-based sensors are made by immobilizing DNA on electrode and backfilling with 6-mercaptohexanol (MCH), forming a self-assembled monolayer, and detecting the electrochemical signal of a redox molecule attached to the DNA molecule. This signal is enhanced or repressed upon binding of an analyte of interest to the DNA. The Easley group have developed several sensors with detection in the pM to nM range on different immuno-assays, including quantification of testosterone and its antibody. However, although this sensor has shown improved sensitivity, the working conditions, such as the inter-oligonucleotide spacing at the microscopic level, are likely far from optimum as the surface characteristics of the sensor are yet to be studied and optimized. The present study employs atomic force microscopy (AFM) imaging to characterize the sensors surface and square wave voltammetry (SWV) to determine current signal. The study also investigates the effect of annealing of the gold-on-glass electrode used for bowtie sensor fabrication at high temperatures. Investigations are done at every step of the sensors fabrication, using different concentrations of the ligated DNA and MCH, and different immobilization durations. The results show that annealing increased the total roughness of the electrodes (RMS roughness (Sq): Unannealed = 8.61 nm; Annealed = 11.37), reduced the current by half, and lead to peeling of the gold electrodes from the glass. Understanding bowtie sensors surface characteristics will lead to the optimization of the sensor parameters leading to improved sensitivity and other performance characteristics. By extension, the results would be applicable to the optimization of any DNA monolayer-based electrochemical sensors.

## Olaniyan, Joseph – Graduate Student, Auburn University

**Authors:** Joseph Olaniyan, Evangelos Miliordos
**Title:** Ab-Initio Study of Methane Activation by Metal Anions.

**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. Specifically, we perform Density Functional Theory (DFT) calculations to investigate the reaction of methane with Cu, Co, Ag, and Au. We optimized the geometries of adsorbed species as reactants, transition states, and the various possible products. Our results show that Cu and Co can form

stable HCuCH3 and HCoCH3 compounds, albeit via high activation barriers, while Ag and Au cannot. These observations are in agreement with the experimental photoelectron spectra recorded for the products of the studied reactions. All calculations were performed using Gaussian 16 with the exchange-correlation functional B3LYP and the aug-cc-pVTZ basis sets. Relativistic effective core potentials were used for Au and Ag combined with the appropriate aug-cc-pVTZ-PP basis sets. Vibrational frequency calculations were used to confirm that the transition states bear a single imaginary vibrational frequency, and that reactants and products bear only real vibrational frequencies.

## Ro, David – Undergraduate Student, Auburn University

**Authors:** Wen Xue, Taesung Kim, Bin Duan, David Seung-Hyun Ro
**Title:** A Facile Strategy for the Fabrication of Cell-Laden Porous Alginate Hydrogels based on Two-Phase Aqueous Emulsions

**Abstract:** Porous alginate (Alg) hydrogels possess many advantages as cell carriers. However, current pore generation methods require either complex or harsh fabrication processes, toxic components, or extra purification steps, limiting the feasibility and affecting the cellular survival and function. In this study, a simple and cell-friendly approach to generate highly porous cell-laden Alg hydrogels based on two-phase aqueous emulsions is reported. The pre-gel solutions, which contain two immiscible aqueous phases of Alg and caseinate (Cas), are cross-linked by calcium ions. The porous structure of the hydrogel construct is formed by subsequently removing the Cas phase from the ion-cross-linked Alg hydrogel. Those porous Alg hydrogels possess heterogeneous pores 100 μm and interconnected paths. Human white adipose progenitors (WAPs) encapsulated in these hydrogels self-organize into spheroids and show enhanced viability, proliferation, and adipogenic differentiation, compared to non-porous constructs. As a proof of concept, this porous Alg hydrogel platform is employed to prepare core-shell spheres for coculture of WAPs and colon cancer cells, with WAP clusters distributed around cancer cell aggregates, to investigate cellular crosstalk. This efficacious approach is believed to provide a robust and versatile platform for engineering porous-structured Alg hydrogels for applications as cell carriers and in disease modeling.

## Uwamahoro, Hilarie – Graduate Student, Tuskegee University

**Authors:** Hilarie Uwamahoro, Willard E. Collier, Toufic O. Nashar, Desmond G. Mortley, Jesse M. Jaynes and Cheryl G. Davis
**Title:** Cyclic Peptides as Potential Antiviral Drugs to Combat Future Pandemics

**Abstract:** The emergence of SARS-CoV-2 and its variants has exposed the urgent need for new specific and broad-spectrum antiviral drugs. Medicinal plants represent a vast source of bioactive compounds, including cyclic peptides, which have shown potential as antiviral agents. Cyclic peptides from medicinal plants as new antivirals are a relatively new field and their full potential has not been explored. Our

research aims to identify and characterize antiviral cyclic peptides from the seeds of Hibiscus sabdariffa (hibiscus), Cannabis sativa (industrial hemp), Abelmoschus esculentus (okra), and Ocimum basilicum (basil). The plants were grown at George Washington Carver Experimental Farm and the seeds were collected, dried, and ground. The protein content of the ground hemp, hibiscus, and okra seeds was determined using the Kjeldhal method. Our results found that they contained 513 mg/g, 373 mg/g, and 377 mg/g of protein, respectively. The protein isolates of the three seeds were obtained using standard protein isolation methods. The protein concentration of each isolate determined using a Protein A280 application on a NanoDrop Eight Spectrophotometer was 106 mg/ml in hemp, 92 mg/ml in hibiscus, and 499 mg/ml in okra. The protein isolates were analyzed using sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS PAGE). The SDS PAGE revealed distinct bands representing proteins of approximately 48KDa, 35KDa, 24KDa, 22KDa, 20KDa, and 10KDa. Separation and characterization of cyclic peptides in the protein isolates is ongoing. Future work will include antiviral inhibition assays and molecular modeling studies of isolated cyclic peptides. This project promises to advance antiviral drug development and contribute to the global fight against viral infections.

## Zhan, Ke – Graduate Student, Auburn University

**Authors:** Ke Zhan, Thomas Elder, and Yucheng Peng
**Title:** Enhancing polypropylene/high-density polyethylene blend performance with microcrystalline cellulose-based core-shell structure particles at the interface

**Abstract:** Enhancing the performance of polypropylene (PP)/high-density polyethylene (HDPE) blend is crucial for valorizing mixed plastic waste. This study incorporated microcrystalline cellulose (MCC), combined with maleic anhydride grafted polyethylene (MAPE), into the PP/HDPE blend to enhance its performance. Mechanical results showed that the addition of MCC increased strength, stiffness, and toughness of the PP/HDPE blend, with further enhancement achieved through adding MAPE. Morphological observations and thermal analyses revealed that the enhanced mechanical properties were attributed to the formation of core-shell structure particles, with MCC as the core and MAPE, miscible with HDPE, acting as the shell at the interface. These MCC-based core-shell structure particles demonstrated great potential for improving the PP/HDPE blend performance.

**Lodging Information (Recommendation)**

Hampton Inn Columbus Downtown – 1201 Broadway, Columbus, GA 31901

**Parking Information (All recommended lots are free)**

Rivercenter garage (916 Front Avenue, Columbus, GA 31901) or the Dillingham parking lot adjacent to it. You will cross Front Ave to enter the Bo Bartlett Center.

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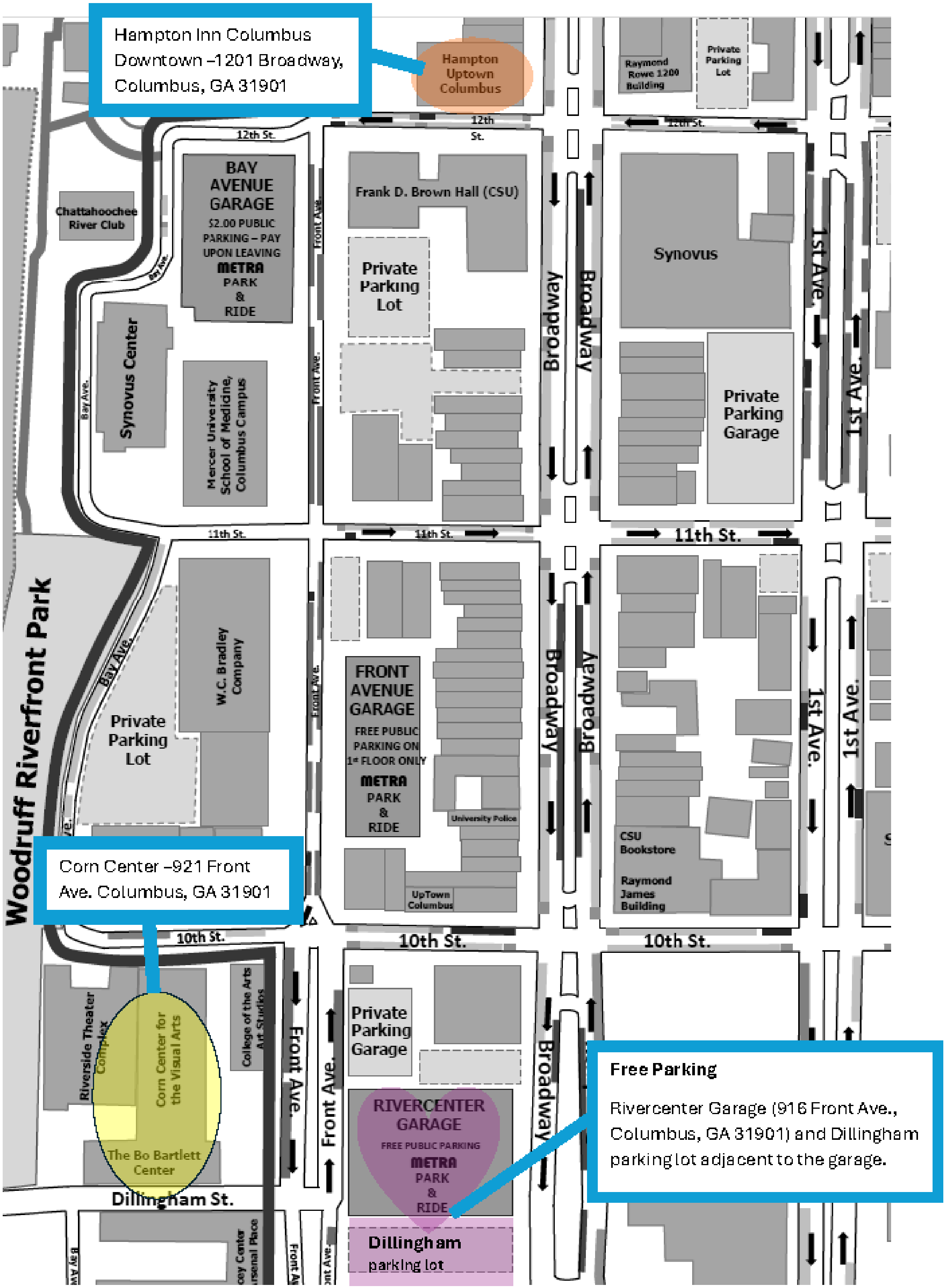
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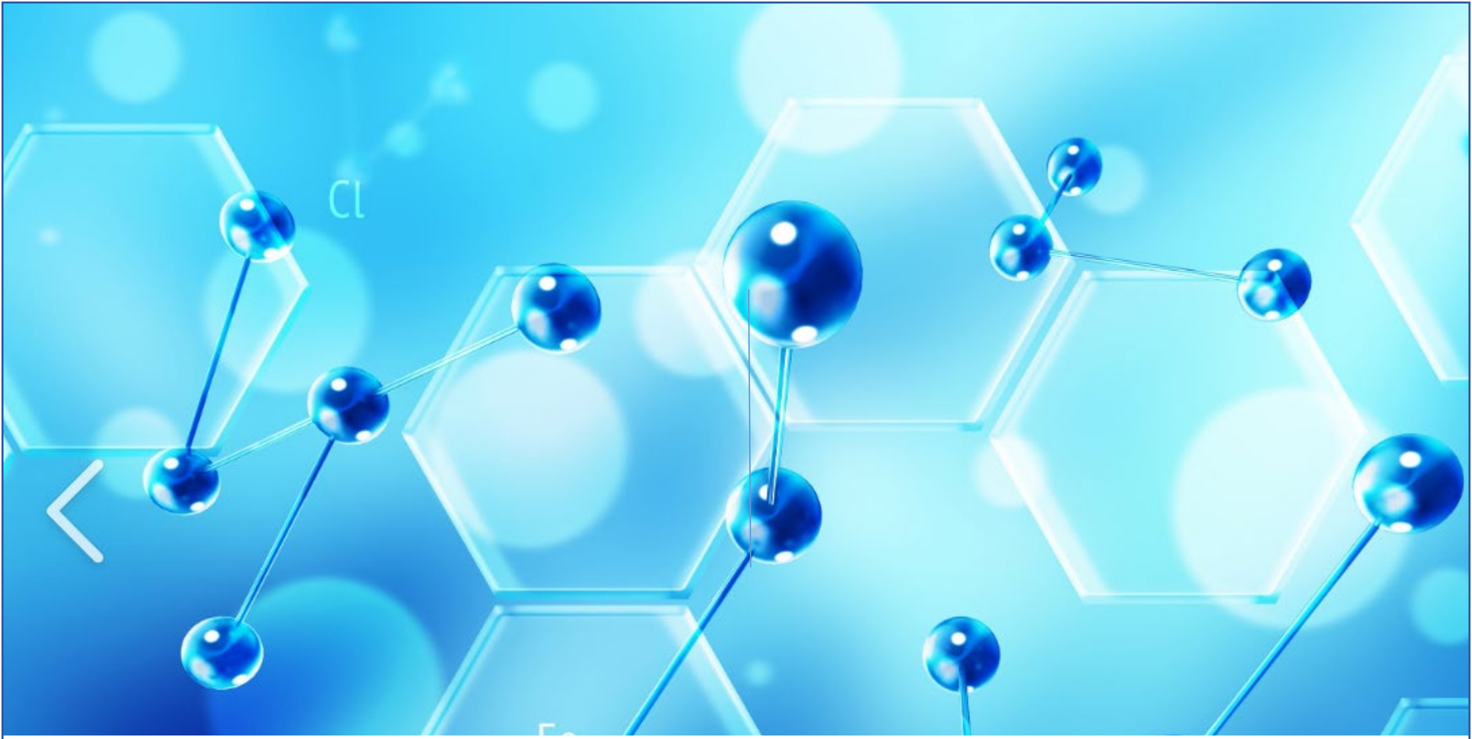

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