Oral Presentation Abstracts

For presentation times, please see the schedule.

Advanced Mass Spectrometry-Based Lipidomics Using Dual-Source timsTOF Technology

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Leveraging dual-source timsTOF technology, I investigated lipid structural characterization and spatial distribution in the brain of an Alzheimer's rat model. The study utilized Reverse Phase Liquid Chromatography Tandem Mass Spectrometry (RPLC-MS/MS) coupled with trapped ion mobility spectrometry (TIMS) to enhance lipid separation, detection, and annotation. We obtained more mass spectral features and thus annotated more lipids in timsON mode compared to timsOFF, thanks to improved separation of lipid isomers and higher-quality tandem spectra. I employed Bruker MetaboScape and open-access MS-Dial software for data processing and compound identification. Ultimately, LC-MS/MS with timsTOF enhanced both the quantity and quality of features in untargeted lipidomics. Additionally, Matrix-Assisted Laser Desorption Ionization (MALDI) Mass Spectrometry was used to image the AD rat brain. Building on lipid structural insights from the LC-MS/MS analysis, I annotated lipids and visualized their spatial distribution in the Alzheimer's transgenic rat model compared to wild-type controls. Distinct spatial patterns were observed for glycerophospholipids, ether lipids, and sphingolipids in the brain. Together, these studies demonstrate the power of mass spectrometry technology in lipidomics research, providing new insights into lipid characterization and visualization.

Investigating The Effect of Post-Translational Modifications on Cu2+ binding to the Antimicrobial Peptide PG-KI

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As antibiotic resistance rapidly increases, the healthcare industry has focused much attention to fighting an emerging antibiotic crisis. Antimicrobial peptides (AMPs) have become a promising alternative to current antimicrobial therapies. AMPs are naturally occurring peptides that contribute to the innate immune system of many organisms. Some AMPs, such as Pseudophryne güntheri Kassinin-1 (PG-KI; EPHPDEFVGLM), have been shown to bind to metals such as Zn(II) and Cu(II) which may aid in their antimicrobial efficacy. PG-KI has a metal binding motif similar to the Amino Terminal Cu(II)

and Ni(II) (ATCUN) binding motif, and has been observed to contain a posttranslational modification (PTM) of the N-terminal glutamate which cyclizes into pyroglutamate (pGlu). Despite the promise of AMPs, little is known about how their structure and peptide efficacy is impacted by the binding of metals. Furthermore, the impact of naturally occurring PTMs on metal-ion binding is poorly understood. This investigation uses isothermal titration calorimetry (ITC) and a variety of spectroscopic techniques show that non-modified PG-KI binds Cu2+ with nanomolar affinity while the pGlu post-translation modification increases the binding affinity into the picomolar range. These results not only offer insight into the metal binding properties of antimicrobial peptides such as PG-KI, but expand our understanding of other metalmodulated peptides with similar PTMs.

Discovering Chemical Determinants of p53 Amyloid Formation

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Protein aggregation into toxic amyloid fibrils underlies diseases including neurodegeneration and numerous cancers. p53 is a critical transcription factor and tumor suppressor protein that regulates a broad range of cellular processes, but has been observed to accumulate in filamentous amyloid aggregates in cancer cells. p53 amyloid formation likely contributes to loss-of-function phenotypes observed in cancer; however, the cellular environmental factors driving transformation of p53 to its amyloid state remain poorly understood. Here, we develop a system to test the chemical determinants of p53 amyloid formation systematically. Using purified recombinant p53, we will explore the potential for components of the cellular environment, including cellular metabolites that are responsible for p53 activity and stabilization. Through Differential Scanning Fluorimetry (DSF) experiments, we are investigating the role of pyruvic acid and 4-hydroxy-4-methyl-2-oxoglutaric acid (HMOG) in inducing p53 stabilization or destabilization. Next, we are also interested in screening endogenous metabolite libraries to study the physiological conditions that facilitate p53 propensity to unfolding or misfolding. We expect that our results will enable mechanistic models of p53 aggregation and inform drug development efforts to prevent p53 loss of function in oncogenesis.

Analyzing Pathology Images with Large Language and Imaging Models

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A traditional biopsy method for investigating cancer suspicious skin tissue, while effective, is invasive and time-consuming, as it involves multiple processing steps to produce

Hematoxylin & Eosin (H&E) stained images, which are the gold standard for cancer diagnosis. In 2021, Winetraub lab introduced a groundbreaking alternative: virtual biopsy, a non-invasive approach to detect skin cancer. This method involves scanning live tissue with an Optical Coherence Tomography (OCT) scanner and using a machine learning-based generative adversarial network (cGAN) to convert the grayscale OCT images into H&E-like virtual images. While virtual H&E images hold great promise as a non-invasive diagnostic tool, ensuring their reliability for clinical use remains a critical challenge. Thus, this study was conducted to determine whether virtual H&E images from virtual biopsy can function as a viable substitute for traditional biopsy in clinical settings. In this research, large language and imaging models, such as GPT-4 and Pathology Language Imaging Pre-trained (PLIP) models, were utilized to analyze OCT scans, paired traditional H&E images, and paired virtual H&E images to evaluate how well models identify skin structures and features in those images. Moreover, we developed a pipeline that uses ResNet50 and UNI (a pathology pretrained image encoder) models to extract feature embeddings (number representations) from 256x256 patches of virtual H&E whole slide images. These embeddings are then compared to those of a reference cancerous tissue patch image that contains Basal Cell Carcinoma skin cancer to detect cancerous regions in virtual H&E images with the use of a cosine similarity technique. We found that GPT-4 and PLIP models accurately identified skin features and structures in around 85% of virtual H&E images. This high accuracy suggests that virtual H&E images from virtual biopsy, combined with AI models, could be a promising non-invasive method for detecting skin cancer. Additionally, we discovered that the UNI model successfully detected cancer areas in virtual H&E images. This highlights virtual H&E images' potential viability as a substitute for real H&E images and underscores the promise of virtual biopsy techniques to detect and diagnose skin cancers non-invasively.

Investigation of the mechanism of Opuntia ficus-indica by fractionation

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There is a growing number of people with undiagnosed and untreated diabetes, especially within underrepresented groups in the United States. Previous research has shown that Opuntia ficus-indica (OFI), commonly known as nopales or prickly pear, has helped reduce blood glucose levels after consumption in diabetic patients. While minimal research has proven the benefits of nopales, the reason as to why and how it has hypoglycemic properties is still being examined. In order to study the effect of nopales on the human body, three goals will be investigated: fractionate OFI in order to determine its hypoglycemic compounds, identify and maintain a cell line to analyze glucose uptake in cells, and observe and quantify the process of the reactions between OFI compounds and glucose within cells via a fluorescent assay. This research project aims to narrow the investigation of the mechanism of Opuntia ficus-indica and its interactions with glucose by

means of fractionation. To do this, various fractions of the plant will be investigated and assayed.

Design, Synthesis, and Surface Exchange Studies of Calamitic Promesogenic Amine Capping Ligands for CdSe/ZnS Quantum Dots

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Quantum dots (QDs) are fluorescent semiconducting nanoparticles that have been used in LEDs and sensors. We have generally used a concise three-step synthetic route to prepare a small library of liquid crystal-like ('mesogenic') primary amine-bearing ligands featuring a rod-like (‘calamitic’) multi-benzene backbone. These ligands have been used to prepare ligand-modified QDs and direct their self-assembly into microstructures. Here we describe our latest ligand designs and synthetic approaches, as well as ligand stability considerations, and an example of how we quantify ligand exchange efficiency using 1H NMR. Understanding the relationship between ligand structure and exchange efficiency will help inform ongoing QD self-assembly studies conducted by our collaborators.

Developing methods to investigate the role of ubiquitin in destabilization and misfolding of the cancer-associated proteins p53 and PTEN

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Ubiquitin is a protein posttranslational modification (PTM) typically appended to lysine residues of substrate proteins to target them for degradation by the proteasome. The model protein Barstar displays differential sensitivity to ubiquitination depending upon the exact site of attachment; ubiquitin destabilizes barstar’s fold when attached to some locations but has no effect when attached to others. However, it remains unknown if these effects occur across the proteome, including for critical signaling proteins like tumor suppressors that are known to be regulated by ubiquitination and misregulated in cancer. Here, we use biophysical methods to measure the effect of ubiquitin on the thermodynamic stability of two tumor suppressor proteins, p53 and PTEN. We have developed biochemical techniques to attach ubiquitin to p53 and PTEN. Using purified ubiquitinated proteins, we systematically analyze the effect of ubiquitin attachment at different locations and the effect of ubiquitin on p53 and PTEN function and proteasomal degradation. To expand these studies, we have also created a Differential Scanning

Fluorimetry (DSF) platform to identify fluorogenic dyes that are specific for individual ubiquitin proteoforms. In this process, we screened a library of dyes to identify hits that specifically recognize monoubiquitin and/or K48- and K63-linked polyubiquitin chains. We envision that these dyes will be useful for rapid detection of ubiquitin proteoforms in biological systems and to monitor protein degradation in real-time in a more accessible manner than protein imaging methods. It is known that p53 and PTEN are often misregulated and lead to the proliferation of cancer; the role of ubiquitin signaling in this misregulation will be crucial to understanding this process thus leading to better treatments. Understanding the patterns of ubiquitination will help identify key enzymes and pathways involved in tumor progression and uncover potential therapeutic targets.

Inhibitory Activities of Surface-Associated Bacteria from California and Florida Algae

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Marine algal surface-associated bacteria (SAB) inhabit highly competitive and diverse marine environments, where they face challenges such as high salinity, osmotic stress, and UV radiation. In response, these bacteria produce secondary metabolites that may serve as chemical defenses, including potential antibiotics active against human pathogens. To discover novel antibiotic drug leads, algae samples were collected from three California beaches (Stinson Beach, La Jolla, and Santa Cruz) and the Florida Keys. SABs were isolated from plates where algal surface swabs were plated on A1 medium, then cultured in liquid A1 medium (10 g/L starch, 4 g/L yeast, 2 g/L peptone), and cryopreserved. We utilized 3 antimicrobial screening methods—pour-over assay, disk diffusion, and single-dose broth assay— to test the 532 isolates against four human pathogens: Escherichia coli, Bacillus subtilis, Staphylococcus aureus, and Salmonella sp. In the pour-over assay, 11 isolates from an initial pool of 332 California SABs and 17 isolates from approximately 200 Florida SABs, produced zones of inhibition indicative of antibiotic production. The disk diffusion assay also confirmed antibiotic production in 14 samples. These antibiotic-producing isolates were then cultured large scale in 500 mL A1 media for 48 hours, extracted using XAD-16 resin, and then the broth was further extracted using ethyl acetate. Single-dose broth assay was conducted on the fractions from the large-scale extracts. The next steps will be isolation and characterization of the antibiotic secondary metabolites.

Investigating Size and Illumination Effects on the Photocatalytic Activity of Quantum Dots and Nanorods

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The global push toward renewable resources has amplified the demand for sustainable alternatives to petroleum-derived chemicals. Biomass valorization through lignin depolymerization offers a promising route to high-value aromatic compounds from nonfossil carbon sources. However, this process often relies on non-selective or expensive catalysts that degrade quickly or require harsh reaction conditions. There is a growing need for catalytic systems that are more efficient and selective. Semiconducting nanomaterials, such as quantum dots (QDs) and nanorods (NRs), are emerging as powerful photocatalysts due to their tunable electronic properties, high surface area, and strong solar harvesting ability. In this work, we investigate the photocatalytic performance of spherical and anisotropic CdSe nanocrystals in driving photolytic reductive cleavage of C–O bonds within lignin model compounds. By systematically varying particle size, shape, and surface ligands, we assess the impact of structural and electronic properties on QD catalytic efficiency and electron transfer dynamics under both white light and monochromatic 365 nm excitation. Interestingly, larger QDs often outperform their smaller counterparts, a trend that runs counter to Marcus theory predictions, which posits that smaller particles with higher redox potentials should be more catalytically active in electron-transfer processes. These findings provide valuable insights into the structure-function relationship of nanoscale photocatalysts for developing more efficient, affordable, and sustainable systems for light-driven chemical transformations.

Utilizing Impedance Spectroscopy to Optimize the Fabrication of Semitransparent Agrivoltaics

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Over the next two decades, rising demands for food, energy, and clean water are expected due to current consumption trends and steady population growth. Agrivoltaic systems, which combine solar energy production with agricultural production in areas with high solar irradiation, offer a creative way to help meet these increasing demands. In previous work, a fully solution-processible method for fabricating semi-transparent solar cells was developed. However, the efficiencies of these research-grade organic photovoltaics (OPVs) reached only 2.95×10-07%. For future greenhouse use, efficiencies of 1-2% are desired. This study investigates the use of circuit analysis to enhance the performance of OPV devices. The thickness of each layer of an OPV device plays a

critical role in determining the device's series resistance, which in turn affects its overall efficiency and performance. By employing Bode and Nyquist plots, the impedance characteristics of OPVs were examined to pinpoint reductions in series resistance before and after adjusting the thickness of the device's layers. For the thickness adjustments of each layer, atomic force microscopy was used to reach the optimal thicknesses for OPV functionality. Furthermore, capacitance and shunt resistance were analyzed in relation to potential recombination effects. The extracted parameters were used to validate experimental methods aimed at reducing series resistance and addressing performance issues, ultimately improving the efficiency of the
OPV devices to 0.05%. Future work will explore the effects shading has on lettuce plant growth using newly constructed evaluation platforms fitted with sensors. Sensor data will be analyzed to compare plant growth under purchased silicon panels, fabricated OPV panels, and full sun. An agricultural specialist would then evaluate the lettuce plants grown under the OPV panels to quantify the economic impact of using semitransparent agrivoltaic systems to grow shade-tolerant crops.

A Modular Platform for Cell Sorting via Sorting by Interfacial Tension (SIFT)

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Cell sorting is an essential step in biomedical research and diagnostics; however, conventional high-throughput methods like fluorescence-activated and magneticactivated cell sorting depend on costly, label-based techniques. Microfluidics–the manipulation of fluids in microscale channels–offers a promising alternative through its utilization of picoliter-scale droplets that require minimal reagent and sample volumes. Sorting by Interfacial Tension (SIFT) is a passive and label-free microfluidic sorting method developed in the Abbyad lab which exploits differences in the acidification rate of an encapsulated cell to select droplets according to their interfacial tension. The existing "in-line" SIFT system (where droplet generation, incubation, and sorting occur sequentially on one microfluidic chip) limits optimal parameter control, reproducibility, and overall sorting throughput due to cumulative flow instabilities and unintended droplet interactions. To overcome these limitations, we developed a modular microfluidic design, partitioning droplet generation, incubation, and sorting into dedicated devices. This modular approach allows each phase to be independently optimized, significantly improving sorting precision by reducing droplet size variability and stabilizing chemical composition, while substantially increasing throughput by removing constraints imposed by upstream processes. This work underscores modular microfluidic design as an effective strategy to advance the scalability and applicability of passive droplet sorting technologies.

CRISPR Screening to Identify E3 Ubiquitin Ligases Responsible for Human Histone Degradation

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Nucleosomes are the fundamental units of chromatin, comprising genomic DNA wound around a histone octamer. This octamer typically consists of two dimers of histones H2A and H2B, and one tetramer of histones H3 and H4. Chaperones move histones in and out of chromatin throughout the cell cycle, with multiple processes contributing to an extra-nucleosomal histone pool. Though histones are normally accompanied by chaperones, free positively-charged histones may bind to cellular structures nonspecifically causing irreparable damage. Unregulated histone levels are often associated with genomic instability, which confers cancer. Despite their cytotoxicity, the mechanism of histone homeostasis in humans is unknown. Evidence suggests that homologous histones in budding yeast are targeted for degradation via the ubiquitinproteasome system (UPS). The UPS is an enzymatic cascade resulting in the multi-monoubiquitination or polyubiquitination of target proteins and the signaling for their proteasomal degradation. Polyubiquitination depends on an enzymatic cascade involving E1 ubiquitin-activating enzymes, E2 ubiquitin-conjugating enzymes, and E3 ubiquitin ligases. E3 ubiquitin ligases are responsible for the selectivity of proteins targeted for degradation and hundreds of enzymes are classified as E3 ubiquitin ligases.

To determine if E3 ubiquitin ligases are implicated in targeting histones for the UPS, we will perform an arrayed CRISPR knockout screen on cells overexpressing histones using an E3 ubiquitin ligase sgRNA library. After knocking out an E3 ubiquitin ligase that targets histones, the histone levels are expected to rise. To observe a change in histone levels, we will establish a stable cell line expressing a bicistronic vector with GFPtagged histones, followed by a T2A self-cleavable linker, and finally mCHERRY. These fluorescent tags would be aggregated in the nucleus at a 1:1 ratio. We will then introduce 3-4 sgRNAs to induce a heritable gene knockout of individual E3 ubiquitin ligases. GFP and mCHERRY fluorescence will then be compared. If GFP fluorescence compared to mCHERRY is the same, we may assume that the knocked out E3 ubiquitin ligase is not essential for histone degradation. If there is higher GFP fluorescence compared to mCHERRY, it is likely that the E3 ubiquitin ligase plays a role in targeting histones for degradation by the proteasome.

Ruthenium complexes bearing a chemically non-innocent pincer ligand: a tunable system with potential to promote alkyne-centered reactivity

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The coordination of an alkyne to a transition metal complex may facilitate novel reactivity and the stabilization of unusual intermediates, particularly if the alkyne is incorporated into a multidentate ligand that provides structural rigidity. Inspired by the stabilization of cyclobutadiene by iron and other metals, the Deegan lab has targeted metal-alkyne systems as candidates for accessing other strained, anti-aromatic heterocycles such as oxirenes, thiirines, and 1-H azirenes. “PCCP” ligands are known to bind to metals through their two phosphine donors and alkyne, have been sterically and electronically modified at their aryl rings and phosphines, and may be characterized by 31P NMR. Alkyne-centered reactivity may be promoted by the coordination of PCCP to low spin, d6 metals, which tend to be slow to undergo ligand substitution. To this end,
I synthesized the novel ruthenium (II) complex mer-(PCCP) RuCl2PPh3 and investigated its reactivity with RN-group, O-atom, and S-atom transfer reagents. Rather than the desired alkyne-centered transformations, the complex exhibited reactivity at the bound triphenylphosphine. Upon exposure of the triphenylphosphine complex to cyclohexene sulfide, clean conversion to mer-(PCCP)RuCl2(C6H10S) was observed. Potential methods for tuning the metal-alkyne system to favor ligand-centered reactivity over metal-centered reactivity will be discussed, along with efforts to synthesize and characterize ruthenium-PCCP complexes at different oxidation states.

Decoding H3.3 Variant Nucleosome Interactome

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The human genome is packaged within the nucleus as chromatin, a polymeric structure composed of repeating units called nucleosomes. Each nucleosome contains approximately 150 base pairs of DNA wrapped around a histone octamer, consisting of two copies of each canonical histone H2A, H2B, H3, and H4. Canonical histones are biosynthesized during DNA replication; however, there also exists variant histones that can replace their canonical counterparts and be expressed throughout the cell cycle. Due to their distinct amino acid composition, variant histones alter chromatin's chemical and physical properties, influencing protein interactions during genome-templated processes. Variant nucleosomes can include two identical variant histones (homotypic) or a combination of one variant and one canonical histone (heterotypic). Mutations of variant histone H3.3 have been correlated to various cancers. My research addresses a critical gap in understanding the mechanisms regulating heterotypic H3.3/H3 and homotypic

H3.3 variant nucleosome interactions with nuclear proteins compared to their canonical counterparts. I have already reconstituted homotypic H3.3 nucleosomes and aim to reconstitute the heterotypic H3.3/H3 types, which is technically challenging due to ensuring precise incorporation of specific variant histones at defined positions. I intend to follow a recent study that developed a traceless method to synthesize canonical nucleosomes containing different posttranslational histone modifications on each histone H3. To date, I have introduced mutations into histone H3.3, for expression and purification. The next step involves assembling tetramers containing both mutated H3.3 variant and canonical H3 through chemical crosslinking to establish heterotypic configuration, which will subsequently be used for reconstituting heterotypic nucleosomes. By establishing an efficient method for assembling variant histone octamers, I will reconstitute H3.3 into heterotypic variant nucleosomes to incorporate into our nucleosome library. The nucleosome library with varying histone combinations will be used in a comprehensive proteomic screen with human cell nuclear lysates to identify protein complexes that preferentially interact with variant histones in each configuration. Identifying variant-specific nucleosome interactions provides a unique opportunity for identifying potential anticancer therapeutics that target cells with H3.3 dysregulation.

Deciphering the Acidic Patch Interactions of Human H2A.Z Variant Nucleosome

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Eukaryotic genes are tightly packaged in a polymeric complex called chromatin. The fundamental units of chromatin, nucleosomes, are assembled with ~150 base pairs of DNA wrapped around eight histone proteins, consisting of two H2A/H2B dimers and an H3/H4 tetramer. These histones are classified as replication-dependent because their expression is coupled with DNA synthesis during the S-phase of the cell cycle. The histone core has been shown to interact with many nuclear proteins, revealing the dynamic role of nucleosomes in cellular processes. Moreover, the H2A acidic patch, an area of negatively charged amino acids, has been shown to be a hot-spot for nuclear protein interactions. H2A.Z, a variant of histone H2A, is independent of replication, expressed throughout the cell cycle, and has a different amino acid sequence that leads to its unique function. H2A.Z regulates numerous cellular processes: embryonic development, neuronal development, and brain function. Interestingly, H2A.Z contains one more acidic residue in the acidic patch compared to its canonical counterpart, suggesting a possibility for distinct interactions.

Our lab aims to establish a library of nucleosomes that will include canonical and variant histones to study how nuclear proteins recognize them. We have expressed two acidic patch mutants in BL21 (DE3) pLysS cells that (i) neutralize the acidic patch and (ii) introduce a phosphomimetic mutation that increases the nucleosome acidity. Dimerization of mutated H2A.Z with H2B and reconstitution with biotinylated DNA using gradient salt dialysis has yet to be done in preparation. Nucleosomes will be incubated

with cell nuclear lysates to perform a pulldown assay, and the bound proteins will be analyzed using quantitative mass spectrometry. Data gathered will be compared to canonical nucleosomes, revealing protein interactions affected by H2A.Z acidic patch mutations. By identifying disrupted nucleosome binding patterns of proteins that contribute to disease progression, we have the potential to reveal new therapeutic targets.

Kinetics of Methylglyoxal Oligomer Reactions Driven By Dilution During Cloud Droplet Formation on Aerosol Particles

Mateo Johnson, Esmeralda Mendoza Corrales, Brian Ta, Kimberly Houghton, Rasha Alnajjar, Weston Schweitzer, Annalise Van Wyngarden

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Aerosol particles have complex effects on climate, through cloud formation and radiative absorption/scattering. These climate forcing properties can be altered by chemical changes during cloud formation/evaporation on aerosols. For example, the speciation of methylglyoxal oligomers in atmospheric aerosols may be altered by cloud formation, since the process causes changes in pH and water activity that may drive hydration, hydrolysis, and/or polymerization reactions. To examine these reactions, the rapid water uptake during droplet formation was simulated by approximately 100-fold dilution of 40 wt.% methylglyoxal and then monitoring of changes in chemical speciation over time with high-resolution quadrupole-TOF mass spectrometry. Multiple masses of each oligomer were observed due to hydration of either monomer precursors or of the oligomers themselves. Results showed that overall polymer kinetic behavior was consistent with sequential decomposition from large oligomers to smaller ones and eventually to monomers. Nonetheless, methylglyoxal oligomers up to the octamer persisted after the dilution. Many oligomers showed initial exponential decay for which rate constants are reported. Individual oligomer concentrations continued to change for 20 minutes to 4 hours after dilution, exceeding a typical cloud droplet lifetime (~10 min.). Therefore, the kinetics of these speciation reactions should be considered in modeling the impact of cloud formation on organic aerosols.

Analysis of Ion Binding Constants of a Three-Fold Symmetric Copper Complex

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This project aims to determine the binding efficacy of a copper complex host to an inorganic phosphate guest, primarily by identifying the reaction’s thermodynamic equilibrium constant. We hope that this complex, once fully understood, may serve as an

ecologically-sound binder for phosphates in surface water. The three-fold symmetric copper complex supported by N,N-{2-Bis[2-(3-amino-butylamino)ethyl]aminoethyl}-1,3propanediamine, [Cu(TAL)]2+,was first reported by the group of García-España and isolated in our group during the summer of 2024. We are analyzing the selectivity of the [Cu(TAL)]2+ complex towards phosphates in the presence of other common aqueous ions, such as chlorides, sulfates, and nitrates, to better understand this molecule's potential for phosphorus re-capture. In this presentation, we will discuss the experimentally determined equilibrium constants of the host/guest binding of the complex with phosphate and fluoride. The equilibrium constants were determined by titration experiments monitored using UV-vis spectroscopy.

Decoupling Composition and Performance: Single-Source Precursor Design for HighEfficiency Near-Infrared-Emissive Quantum Dots

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Near-infrared (NIR)–emissive colloidal quantum dots (QDs) hold promise for emerging optoelectronic and energy applications, yet their optical performance remains constrained by surface and interface defects. Indium arsenide (InAs) QDs, in particular, exhibit low photoluminescence quantum yield (PLQY) unless effectively passivated with a shell material such as indium phosphide (InP). Traditional shelling protocols employ separate phosphorus and indium precursors, often resulting in inconsistent shell morphology and modest optical gains. In this work, we investigate a single-source precursor strategy for InP shell growth that enables tightly coupled indium and phosphorus delivery under controlled conditions. Surprisingly, microwave plasma– atomic emission spectroscopy (MP-AES) reveals that both single-source and dualsource methods achieve similar phosphorus incorporation. However, only the singlesource route leads to a dramatic enhancement in PLQY, underscoring that elemental uptake alone does not determine optical quality. These results highlight how precursor design fundamentally influences shell formation pathways, exciton dynamics, and ultimately, material performance. Our findings establish single-source chemistry as a powerful tool for modulating nanocrystal interfaces and advancing next-generation NIRactive QDs.

Dilution-Driven Speciation Changes in Glyoxal Polymers During Cloud Formation on Aerosol Particles

Mateo Johnson, Alejandro Municio, Esmeralda Mendoza Corrales, Kimberly Houghton, and Annalise Van Wyngarden

Atmospheric aerosols influence climate by interacting with radiation (scattering and/or absorbing) and by serving as nucleation sites. Glyoxal polymers are common components of atmospheric aerosols. Upon dilution during cloud formation, glyoxal can undergo hydration, hydrolysis, and polymerization reactions, potentially altering the aerosol properties and their climate impacts. It is unknown which polymers decompose on the timescale of typical cloud droplet formation and evaporation. Therefore, water uptake during cloud formation was simulated through a 100-fold rapid dilution of 40wt% glyoxal, and the speciation and kinetics were monitored via high-resolution QTOF Mass Spectrometry. Overall, results indicated the decomposition of larger glyoxal polymers into smaller polymers and monomers post-dilution. Furthermore, polymer speciation changes continued for hours after dilution, indicating that the timescale for many polymer reactions is substantially longer than typical cloud droplet lifetimes. Therefore, polymer speciation reaction rates should be taken into account in future modeling of chemical changes in aerosols during cloud formation.