RESEARCH SYMPOSIUM

Room 310 Poster Session 4 Abstracts

Ciara Aumend

(Diversity) Oral Microbiome and HIV in Children

Previous studies have shown that children living with HIV (CLWH) are more prone to dental caries which may in part be due to a decrease in overall saliva production and changes in the oral microbiome. We hypothesized that the biodiversity of the oral microbiome on incisors and molars would become more amalgamated in CLWH due to the low saliva production inherent in this chronic disease. We compared molars and incisors because previous studies have shown that the oral microbial communities change based on location in the mouth and amount of saliva production.

We examined 110 supragingival plaque samples collected from 108 children living in Nigeria, an underrepresented group in the world of oral microbiome studies. Of the 108, 35 are CLWH, 39 are perinatally exposed to HIV but are uninfected (HEU), and 36 children are unexposed and uninfected (HUU). We used a novel sequencing technique to characterize the microbial community of each plaque sample, then compared the community composition and diversity of molars and incisors in each group.

We found that both HUU and HEU children show statistically significant differences between molars and incisors. CLWH, however, exhibit no statistically significant difference between the two tooth types. This study is part of the first large-scale study of the oral microbiome of CLWH in sub-Saharan Africa, and our results suggest that HIV infection and decreased salivary flow homogenizes the oral microbiome, which may contribute to the increase in dental caries observed in this cohort.

Allison Mann

(Industry) Human Microbiome, Probiotics, Oral Health and Disease

Tooth decay is the most common preventable chronic disease, globally affecting more than two billion people, most of whom are children. The development of caries on teeth is primarily a consequence of acid production by cariogenic bacteria that inhabit the plaque microbiome. Acid sensitive bacteria can counteract environmental acidification and, therefore, caries development, by producing ammonia using the arginine deiminase metabolic pathway (ADS). Given the potential protective capacity of ADS competent bacteria, the exploitation of these microbes through pre- or probiotic treatments is a promising therapeutic target for the prevention of tooth decay, yet the pervasiveness and rate of expression of ADS in diverse mixed microbial communities in oral health and disease remains an open question. In this study, we used a multi-omics approach to characterize the microbial community and ADS expression in health and late-stage cavitated teeth. Results from this study identify potential candidates for probiotic panel development including oral bacteria where pH modulation through the ADS pathway have previously been described (e.g., Streptococcus sp.) as well as those that are less well characterized (e.g., Leptotrichia sp.). In addition, our results highlight the importance of accounting for taxonomic shifts in the interpretation of functional differences in mixed microbial ecosystems and suggests that probiotic development may benefit from further strain-level investigations for ADS activity and pH modulation potential in mixed microbial communities.

Shanna L. Estes

(Environment) Actinide Chemistry

Vis-NIR Spectroscopy for Analysis of Aqueous Neptunium-Acetate Complexation and Thermodynamics

Defining the thermodynamics of aqueous actinide complexation is crucial for understanding the behavior of actinide elements in complex and extreme systems, ranging from contaminated natural and engineered environments to nuclear separations processes. This presentation describes recent efforts to define the stoichiometry and stability of aqueous neptunium (Np) acetate complexes that are expected to form in engineered subsurface nuclear waste repositories. Currently available thermodynamic data disagree on the stoichiometry, stability, and enthalpy of aqueous Np-acetate complexes, such that there is no one set of thermodynamic constants available to model and predict this chemistry. This work uses a new high-resolution UV-Vis-NIR spectrophotometer, acquired via funding from the Clemson University Major Research Instrumentation R-Initiative program, to probe the aqueous Np-acetate system across a range of ionic strengths (0.5–9 m NaCl) and temperatures (25–65 °C). Future work will combine the data obtained using Vis-NIR spectroscopy with data from complementary techniques, including isothermal titration calorimetry, to fully define the thermodynamics of Np-acetate complexation.

Sagar V. Kanhere

(Environment) Carbon Fiber Processing, Composites and Polymer Processing

Carbon fibers are known for their high specific strength and modulus, however, most of the carbon fibers in market are produced from polyacrylonotrile (PAN). PAN is expensive and fiber spinning process involves use of toxic solvents. In this study, we used lignin recovered from corn stover, a large ago-residue, to produce lignin-based carbon fibers. Carbon fibers display tensile strength of 0.95 ±0.12 GPa whereas tensile modulus is about 78 GPa, exceeding the typical glass fiber modulus of 70 GPa.

Qiushi Chen

(Environment) Computational Mechanics; Numerical Modeling of Granular and Porous Materials (geomaterials, lunar and martian regolith, biomass feedstocks); Material Processing and Handling

Porosity is a fundamental material property that effectively dictates the bulk physical, thermal, and mechanical properties of lignocellulosic biomass. In this work, a novel X-ray CT-based quantitative porosity analysis method is proposed, and the developed toolkit is applied to characterize the internal porosity distribution of loblolly pine. In addition, experiment-informed discrete element models have been developed to simulate the mechanical and flow behavior of biomass in support of material preprocessing and handling operations in bioenergy conversion applications.

Maryelle Nyeck

(Environment, Industry, Learning) Deep Eutectic Solvents

Deep eutectic solvents, also known as DESs are a modern class of solvents that have gained attention for their versatility and unique properties in different applications in fields such as green chemistry, biotechnology, and material science. Hydrogen-bonded DESs are defined as a class of ionic liquids that are formed due to the mixture of two or more hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) components in specific stoichiometric ratios which result in a homogeneous liquid with a low melting point, high solubility, and unique chemical and physical properties. The interaction between the HBD and the HBA disrupts the lattice structure of the individual components, consequently lowering the melting point and creating a homogeneous liquid from the hydrogen bond interactions. Identification of these liquids as “deep” eutectics is made when the observed melting point of the liquid is lower than the predicted melting point of the mixture, as calculated using enthalpic data of the individual components. Because of their low melting points and high solubility, DESs can be more attractive than other solvents such as organic solvents and water for specific chemical reactions or applications. The design of new DESs, and DESs that may exhibit different solvating properties in an area of significant interest.

One approach that our group as used is to leverage the similarity of halogen bonding to hydrogen bonding to form new DESs where halogen bonding interactions are prevalent. Halogen bonding is defined as a non-covalent interaction between an electronegative halogen atom and the center of a positive charge or electron deficiency which is found in the neighboring molecule or ion. Halogen bonding can occur between halogen atoms (fluorine, chlorine, bromine, and iodine) and electron-rich atoms or functional groups (other halogens, nitrogen, oxygen, and sulfur atoms). This can be viewed as similar to a hydrogen bond donor such as amines or carboxylic acids interacting with a hydrogen bond acceptor to form a homogeneous liquid. The presence of halogen bonding in DESs has the capability of increasing the stability and improving the solubility of DESs, particularly towards hydrophobic systems.

The current study aims to test combinations of molecules and salts that have various capabilities towards hydrogen and halogen bonding for the formation of eutectic versus cocrystalline products. These products will then be characterized by appropriate techniques (thermal analysis, single crystal X-ray diffraction, Raman spectroscopy, etc.), depending on their form of matter, to identify the specific intermolecular interactions involved in their formation. A longer-term goal seeks to develop a library of eutectic- and crystal forming combinations that can form the basis of predictive models using machine learning approaches.

Madhushi Bandara

(Industry) Halogen Bonding

Exploring halogen bonding in cocrystals and deep eutectics

Authors: Madhushi Bandara1, Arianna Ragusa, Khadijatul Kobra, Hampton Warner, Victoria Critchley, Audrey Gasque, Colin D. McMillen,* William T. Pennington*

Halogen bonding is a noncovalent intermolecular interaction formed between an electrophilic region of a halogen atom (sigma hole), known as a halogen bond donor in a molecular entity which arises due to the anisotropic electron density distribution and a nucleophilic region of another molecular entity, known as a halogen bond acceptor1. Halogen bonding is widely known as a highly directional and tunable interaction. Heavier halogens like bromine and iodine are less electronegative and highly polarizable. A stronger sigma hole can be achieved in these heavier halogens by incorporation of electron-withdrawing groups, such as fluorine with the molecule. Therefore, organoiodines like 1,2-diiodotetrafluorobenzene, 1,3-diiodotetrafluorodbenzene are identified as good halogen bond donors2. The organoiodine molecules can connect the halogen bond acceptor molecules through halogen bonding into larger discrete units, chains, sheets, or frameworks. Halogen bonding interactions are widely utilized to form polymeric networks, improve the lipophilicity of drugs, and enhance the penetration through lipid membranes, and also are one of the key interactions in crystal engineering (rational crystal design)3.

The halogen bonding interactions between acceptors and donors do not always form crystalline materials instead they may result in liquids. Deep Eutectic Solvents (DES) are solvents of a mixture of two or more components at ambient temperature with a much lower melting/freezing temperature than that expected for a mixture of the individual components4. DESs based on hydrogen bonding are already widely explored in the literature but very little work on DESs based on halogen bonding has been reported5,6.

Here, we report the halogen-bonded DES study tetraalkylammonium triiodides (tetrahexylammonium triiodide and tetrapentylammonium triiodide) and organoiodines (1,2 diiodotetrafluorobenzene and 1,3 diiodotetrafluorobenzene). The study of the physical properties of various component ratios and comparison of these DESs with similar cocrystals will be discussed.

References

1. Lisac, Katarina, Sara Cepić, Mirta Herak, and Dominik Cinčić. "Halogen-Bonded Co-Crystals Containing Mono-and Dinuclear Metal-Organic Units: Three-Component One-Pot Mechanosynthesis, Structural Analysis and Magnetic Properties." Chemistry-Methods 2, no. 4 (2022): e202100088.
2. Peloquin, Andrew J., Khadijatul Kobra, Yuxuan Li, Colin D. McMillen, and William T. Pennington. "Halogen Bonding of Organoiodines and Triiodide Anions in (NMe3Ph)+ Salts." ChemPlusChem 86, no. 4 (2021): 612-621.
3. Peloquin, Andrew J., Colin D. McMillen, Scott T. Iacono, and William T. Pennington.

"Halogen and chalcogen bonding between the triphenylphosphine chalcogenides (Ph3P= E; E= O, S, Se) and iodofluorobenzenes." ChemPlusChem 86, no. 4 (2021): 549-557.
4. Martins, Mónia AR, Simão P. Pinho, and João AP Coutinho. "Insights into the nature of eutectic and deep eutectic mixtures." Journal of Solution Chemistry 48 (2019): 962-982.
5. Peloquin, Andrew J., Jena M. McCollum, Colin D. McMillen, and William T. Pennington. "Halogen bonding in dithiane/iodofluorobenzene mixtures: a new class of hydrophobic deep eutectic solvents." Angewandte Chemie International Edition 60, no. 42 (2021): 22983-22989.
6. Abranches, Dinis O., Nicolas Schaeffer, Liliana P. Silva, Mónia AR Martins, Simão P. Pinho, and João AP Coutinho. "The role of charge transfer in the formation of type i deep eutectic solvent-analogous ionic liquid mixtures." Molecules 24, no. 20 (2019): 3687.

Shreeya Sharma

(Industry) Probiotic and Gut Health

During the first week post-hatch, newly hatched chicks are vulnerable to infection with pathogenic microorganisms due to the incomplete development of their immune system. In this study, we sought to investigate whether in ovo administration of probiotic lactobacilli would modulate the gut-associated immune system of pre-hatched chicks. At embryonic day 18, fertilized broiler eggs were inoculated with four Lactobacillus species, including L. crispatus, L. animalis, L acidophilus, and L. reuteri, either as a single species or in combination. The expression levels of different immune-related genes, including interferon (IFN)-γ, interleukin (IL)-1 β, IL-6, IL-8, IL-10, IL-13, and transforming growth factor (TGF)-β, were measured in the ileum and bursa of Fabricius (the primary site of antibody production in chickens) at different time points post-inoculation. Despite the incomplete development of the embryo’s immune system, L. acidophilus consistently elicited higher expression of immunoregulatory cytokines (IL-10 and TGF-β) and cytokines that mediate and regulate cell- and antibody-mediated immunity, such as IFN-γ (a Th1-type cytokine), IL-13 (a Th2-type cytokine) in the bursa of Fabricius compared to the untreated control group. While IL-10 and IL-6 (a pleiotropic cytokine that plays a role in inflammation and immune regulation) were not expressed at baseline in the ileum of the untreated control group, their expression was variably induced in lactobacilli-treated groups. These findings suggest that in ovo supplementation of L. acidophilus modulates the gut immune responses of chick embryos. Studies are underway to investigate whether lactobacilli induced immune responses confer protection against infection with enteric pathogens post-hatch.

Tanuj Gupta

(Industry) Nanomaterials

Silica is one of the most abundant substances on Earth. Chemically expressed as SiO2, silica exhibits a complicated phase diagram with multiple crystalline structures (polymorphs) at different temperature and pressure conditions. Under a shock impact, a significant amount of energy is effectively absorbed due to the phase transition of fused silica to stishovite, thereby taking most of the destructive energy away from these structures. Therefore, it is crucial to have a reliable method to investigate the mechanism behind the phase transition between fused silica and stishovite to better adapt this material as energy absorption and protection materials for future combat protection applications. In this work, the multi-scale shock technique (MSST) method is characterized to study the shock impact of fused silica. The BKS potential is employed to define the interatomic potential of fused silica. We calibrated two artificial MSST parameters, Q and tscale, concerning the simulation box size. We revealed the impact of cutoff radius rc on fused silica's phase transition under various shock velocity conditions. We found that the selection of rc in the BKS potential influences stishovite's nucleation, formation, and growth at different shock velocity conditions. Future work will expand the MSST method to eliminate the parameter calibration and better predict the material behavior under shock impact.

Cecilia Delgado Solorzano

(Society) Human-Centered Artificial Intelligence

Crowdsourcing platforms gather people from different backgrounds to work on the completion of microtasks. The workers on those platforms are presented with tasks defined by requesters from all over the world. The tasks are defined in multiple languages, with English being the predominant language. It is unclear how language barriers can affect workers whose primary language is not English while completing tasks. In this paper, we study their practices and the impact of AI-powered tools on the completion of microtasks. We conduct a pre-test test field experiment in which workers share their current experience with the platform and receive basic training in the use of AI-powered tools. After a week, workers provide feedback on their practices and experiences. We find that workers who complete tasks in their primary language report less confidence in completing

English tasks, and in general, workers perceive the use of the tools as a language-learning mechanism. We aim that the understanding of language barriers in crowd markets can promote more inclusive work conditions.