Applied Surface Science
Room 209 B W - Session AS+BI+CA-MoM

The Power of SIMS

Moderators: Alexander Shard, National Physical Laboratory, **Tanguy Terlier**, Rice University

8:45am **AS+BI+CA-MoM-3 Inspection of Next Generation EUV Resists with NP-SIMS**, ***Markus Langner***, *Gregrey Swieca,* California State University Northridge*; Won-Il Lee, Shixian Ha,* Stony Brook University/Brookhaven National Laboratory*; Nikhil Tiwale, Chang-Yong Nam,* Brookhaven National Laboratory*; Michael Eller,* California State University Northridge

The rapid advancements of the semiconductor industry demand constant innovations at every step of the microchip manufacturing process. Due to the recent jump towards extreme ultraviolet lithography (EUVL), novel approaches to photoresists are necessary, since conventional chemically amplified resists (CARs) exhibit poor EUV sensitivity and the photon density of EUV light sources is orders of magnitude lower compared to deep ultraviolet (DUV) sources. As a result of low photon density, the nature of EUVL is more stochastic, which leads to challenges in the photoresist chemistry to yield good critical dimension uniformity (CDU) and line edge roughness (LER). Hybrid resists of an organic polymer infiltrated with an inorganic metal solve the low EUV sensitivity problem while exhibiting improved etch resistance. However, it is necessary to ensure high homogeneity of the infiltration process, since the size of the infiltrated molecular moieties is comparable to the desired critical dimensions. Analytical techniques are often unable to yield analysis of the organic and inorganic components of a sample at the same time, in conjunction with high lateral resolution and can as a result not resolve inhomogeneity in the resist at a necessary spatial scale. Nano-projectile secondary ion mass spectrometry (NP-SIMS) is a mass spectrometry technique involving the stochastic bombardment of the sample using nano-projectiles separated in time and space, instead of a continuous ion beam. Each impact yields an individual mass spectrum resulting from an impact crater with 10-15nm in diameter, which allows statistical analysis of the sample and emitted secondary ions from different impacts and thus different locations. In this work we studied samples of polymethylmethacrylate (PMMA) infiltrated with InOx via vapor-phase infiltration (VPI) and investigated the uniformity of the infiltration process utilizing NP-SIMS experiments. The data suggests that one cycle of VPI yields an inhomogeneous distribution of In in PMMA, which improves with further infiltration cycles. The abundance of In species increases linearly with the number of cycles as well, indicating successful infiltration for each cycle up to four. Cluster species such as In2+, In2O+ display a non-linear increase with infiltration cycles, which leads to the hypothesis, that the amount if infiltrated indium is as desired but it aggregates in small clusters, which could affect pattern performance of the resist. This research is supported by the U.S. Department of Energy Office of Science Accelerate Initiative Award 2023-BNL-NC033-Fund.

9:00am **AS+BI+CA-MoM-4 Diffusion Study of Sodium in Hard Carbon Anode Active Materials Using a Novel in Situ ToF-SIMS Approach**, ***Pascal Dippell***, *David Schaefer, Lysander Q. Wagner, Alexander Weiß, Bernd Smarsly, Marcus Rohnke,* Justus Liebig University Giessen, Germany

The incorporation, transport and storage of Na in hard carbon (HC) anodes play a crucial role in modern sodium-ion batteries (SIBs) and affect their electrochemical performance.Until now,the diffusion mechanism of Na in the HC microstructure hasnot been fully understood.The most prominent model, whichisdiscussed in the literature,is the adsorption-intercalation-filling model, which includes diffusion along an interface of a pore and through the bulk of the HC. Most diffusion studies use electrochemical methods, but their evaluation is limited by overlapping processes in the cell, which prevents a complete understanding of sodium diffusion.[1]

In this work, we developeda new in situ ToF-SIMS approachforthe determination of the microscopic Na diffusion processes in HC. Therefore,we chose a well-defined HC thin film with an ultra-pure Na layeron top as model system, to obtain a precise interface between the twocomponents. For the preparation of theHC|Na model system we connected anNa effusion cell to an ultra-high vacuum (UHV) preparation chamber, which is directly attached to theToF-SIMS analysis chamber. Thisexperimental setup enables a defined preparation ofour HC|Nainterface and,moreover, allows an accurate determination of the diffusion parameters.After a definedtime, theNa diffusioninto HC is stopped by cooling downthe system to −130°C, and the diffusion profiles are preserved.

By SIMS depth profiling, we received complex diffusion profiles thatinclude several transport parameters.The SIMS crater analysis was possible through the use of an implemented SPM. As a result of these depth profiles and additionalfinite element calculations, a separation of the different transport processesbecamepossible.Specifically, we observed coupled Na bulk diffusion, which is a solid-statetransport process, and Na pore diffusion, which occurs along an interface.The proposed diffusion model is complemented by additional experiments, which displayed the structural behavior of the HC thin films. These experiments include infiltration studies with liquid electrolytes and a tracer ion for demonstrating the accessibility of the pore system, as well as high resolution electron microscopy for imaging the structure of the HC.

References

[1]D. Schäfer, K. Hankins, M. Allion, U. Krewer, F. Karcher, L. Derr, R. Schuster, J. Maibach, S. Mück, D. Kramer, R. Mönig, F. Jeschull, S. Daboss, T. Philipp, G. Neusser, J. Romer, K. Palanisamy, C. Kranz, F. Buchner, R. J. Behm, A. Ahmadian, C. Kuebel, I. Mohammad, A. Samoson, R. Witter, B. Smarsly, M. Rohnke, Adv Energy Mater2024, 14.

9:15am **AS+BI+CA-MoM-5 Investigating Ionic Motion in Memristors via Topographically Corrected ToF-SIMS**, ***Jacob Shusterman***, Oak Ridge National Laboratory, USA

Secondary ion mass spectrometry (SIMS) is a powerful analytical technique which combines the benefits of high-resolution mass spectrometry with sub-micrometer lateral resolution to identify the spatial distribution of elements and molecules in a sample. Capable of both two- and three-dimensional (3D) analysis, SIMS enables chemical imaging of surfaces, devices, and bulk materials, proving a valuable tool for material characterization. Recent studies have successfully demonstrated applications of SIMS for the investigation of ionic motion in resistively switchable neuromorphic materials such as memristors. However, interpreting SIMS data, especially for microelectronic and nanoscale devices, can be difficult due to significant surface topography and data complexity. This makes it challenging to draw accurate conclusions regarding material composition or chemical changes (e.g. ionic motion) without addressing these features in native 3D SIMS chemical images. Here, we discuss various methods for topographical correction and reconstruction of SIMS data to study ionic mobility in memristive thin films.

Two prominent categories of data correction methods are considered including purely mathematical based post-processing techniques and multimodal approaches combining SIMS with atomic force microscopy. These methods are further applied to TaO_x/Ta memristors to reveal ionic migration associated with resistive switching. Here, lower switching currents (< 10μA) revealed oxygen ion migration and preserved memristic behavior of the thin film device. Conversely, resistive switching with currents greater than 10 μA revealed titanium ion migration from the bottom electrode resulting in irreversible switching to a high conductive state. This research can help gain knowledge of fundamental phenomena associated with memristive behavior of materials for implementation in new generations of microelectronic devices.

This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility and using instrumentation within ORNL's Materials Characterization Core provided by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

9:30am **AS+BI+CA-MoM-6 Standardless, Semi-quantitative ToF-SIMS using the Full Spectrum Method (FSM)**, ***Nicolas Molina Vergara***, *Camille Edwards, Andrei Dolocan, Filippo Mangolini,* University of Texas at Austin

The accurate quantification of the hydrogen content in materials remains a significant analytical challenge despite its critical importance in determining material performance, stability, and functionality across numerous applications. Currently, only a limited number of techniques—such as hydrogen forward scattering (HFS) and nuclear reaction analysis (NRA)—provide accurate hydrogen quantification measurements, typically achieving relative errors between 3% and 10%. While time-of-flight secondary ion mass spectrometry (ToF-SIMS) offers excellent chemical characterization capabilities, its application for hydrogen quantification has been primarily qualitative due to matrix effect complications and the absence of appropriate relative sensitivity factors. Here, we report the first successful application of the Full Spectrum Method (FSM) for quantitative hydrogen analysis in organic polymers. Despite being documented in fewer than six publications over the past two decades, FSM represents a

promising approach for semi-quantitative ToF-SIMS analysis by exploiting large ion clusters that incorporate numerous neutral atoms, effectively mitigating matrix effects as cluster size increases. We systematically quantified hydrogen content in a series of polymers—polypropylene (C_3H_6), polystyrene (C_8H_8), polyethylene terephthalate ($C_{10}H_8O_4$), and polytetrafluoroethylene (C_2F_4)—achieving a high degree of agreement with their nominal hydrogen composition and further verified by complementary measurements performed on identical samples using reflection electron energy loss spectroscopy (REELS). Our results establish a pathway for standardless, semi-quantitative ToF-SIMS analysis without requiring complementary analytical techniques, significantly enhancing the practical utility of ToF-SIMS instrumentation.

9:45am **AS+BI+CA-MoM-7 AVS Medard Welch Award Talk: High Resolution Molecular Imaging by Mass Spectrometry – The OrbiSIMS Odyssey***, Ian Gilmore,* National Physical Laboratory, U.K. **INVITED**

Nuclear magnetic resonance and high-performance liquid chromatography mass spectrometry are the “gold standards” for molecular identification. However, they have limited spatial information. Conversely, techniques with high spatial resolution such as electron microscopy, have low molecular identification information. Generally, from an analytical perspective, this creates what can be termed the “Molecular Uncertainty Principle”, where the more certain we are about a molecule’s identity, the less certain we are about its localization [1]. This is a frustrating limit for measurements at the frontiers.

In 2017, NPL introduced the OrbiSIMS technology [2] with an objective to simultaneously provide molecular identification and localisation as close to this limit as possible. Since then, the number of OrbiSIMS instruments around the world has increased significantly and the community [https://www.npl.co.uk/mass-spectrometry/orbisims/resources] of users and range of applications has grown. Here we recount the OrbiSIMS odyssey from the original concept to the latest advances in cryo-OrbiSIMS [3,4], illustrated with examples of the applications in advanced materials [5] and life-sciences [6]. In a look to the future, the concept for a quantum detector to boost Orbitrap sensitivity by an order of magnitude will be presented [7].

References

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[2] M K Passarelli et al., The 3D OrbiSIMS-label-free metabolic imaging with subcellular lateral resolution and high mass-resolving power, Nature Methods, 2017. 14 (12): p. 1175

[3]J. Zhang et al., Cryo-OrbiSIMS for 3D molecular imaging of a bacterial biofilm in its native state”, Anal. Chem. 2020, 92, 13, 9008–9015.

[4]C. L. Newell et al, Cryogenic OrbiSIMS Localizes Semi-Volatile Molecules in Biological Tissues, Angewandte Chemie Int. 2020, 59 (41), 18194-18200

[5] G F Trindade et al., Direct identification of interfacial degradation in blue OLEDs using nanoscale chemical depth profiling. Nature Communications, 2023. 14 (1): p. 8066.

[6]F Zani et al., The dietary sweetener sucralose is a negative modulator of T cell-mediated responses. Nature, 2023. 615 (7953): p. 705-711.

[7]PCT/GB2024/050690 - Improved Spectrometer or Imaging Assembly (2024).

10:30am **AS+BI+CA-MoM-10 ASSD Peter Sherwood Award Talk***, David Scurr*[1]*,* University of Nottingham, UK **INVITED**

11:00am **AS+BI+CA-MoM-12 Delineating Spatial Cellular Complexities Using Multi-omics Approach by GCIB-SIMS***, Hua Tian,* University of Pittsburgh **INVITED**

The molecular and cellular microenvironment plays a critical role in determining biological function, multicellular organization, and cell fate. However, delineating multilevel biomolecular interactions within the same tissue or cells remains challenging due to limitations in analytical approaches and sample preparation compatibility.

To address this, we present a multimodal SIMS approach incorporating water cluster ion/C_{60} beams and a cryogenic workflow, enabling untargeted lipidomics/metabolomics imaging (in both positive and negative modes) and targeted proteomics in near-native-state tissue at 1 µm spatial resolution. Combined with neuron-linked computational analysis, this method reveals the biomolecular networks and metabolic states of distinct cell types.

To demonstrate the power of this approach, we imaged liver and skin tissues, integrating metabolites, lipids, and proteins within the same cells to visualize cell-type-specific metabolic variations. Our workflow captures >200 key ions (e.g., lipids and essential metabolites) and identifies diverse cell types (e.g., stem cells, lymphatic cells, immune cells, and senescent cells) in regions such as the liver portal/central vein and hair follicles.

Further computational integration aligns multiomics data with segmented cells for clustering analysis, uncovering metabolic and cellular gradients in the liver and the stem cell microenvironment of hair follicles during aging. This study establishes cryogenic Dual-SIMS as a powerful tool for single-cell multiomics imaging, revealing that metabolic and cellular organization is crucial for tissue and stem cell function.

11:30am **AS+BI+CA-MoM-14 Arsenic Quantification in SiGe: Advancing Accuracy with Orbitrap™-SIMS***, Alexis Franquet,* IMEC Belgium*; Alexander Pirkl,* IONTOF GmbH, Germany*; Rita Tilmann,* IMEC Belgium

For over 50 years, Secondary Ion Mass Spectrometry (SIMS) has been crucial in the microelectronic industry providing precise analysis of dopants and impurities in semiconductors [1]. Initially used for blanket samples, SIMS now must analyze patterned samples due to the shift from 2D to 3D devices to continue to support effective process development and optimization in the Fab. This shift presents challenges, including measuring features smaller than the beam spot size and dealing with complex mass spectra with more and more mass interferences due to increased number of elements present in the devices. As a result, SIMS analysis has become increasingly complex, making it harder to extract precise information about bulk and layer composition, dopant quantification and layer uniformity. To meet this need of ultimate lateral resolution without scarifying sensitivity, innovative approaches like Self-Focusing SIMS (SF-SIMS) have been developed, allowing SIMS to profile dopants and quantify bulk composition of multilayers stacks in very small structures [2]. This advancement is particularly crucial for modern devices that incorporate materials such as SiGe doped with As. However, measuring As in SiGe remains a significant challenge due to strong mass interference between As and GeH signals at mass 75 [3]. This challenge is even more pronounced for low-dose As implantation in small SiGe structures, where conventional SIMS instruments lack the mass resolution required for accurate quantification. In this study, we leverage the cutting-edge Orbitrap mass analyzer in the M6 Hybrid instrument to overcome these limitations. The Orbitrap enables mass resolution of more than 240000, which allows to suppress the mass interference at mass 75. We will assess the ability of the Orbitrap to accurately quantify As in SiGe samples, comparing its detection limits, dynamic range, and overall performance against other mass analyzers, including Time-of-Flight, Magnetic Sector, and Quadrupole systems. We will show how the use of calibration curves for both As and Ge quantification for As:SiGe ranging from 0 to 100 Ge at.%, allows to apply SF-SIMS (in Orbitrap) to quantify accurately As:SiGe lines of less than 20nm wide.

[1] P.K. Chu, Materials Chemistry and Physics, 38(3) (1994) 203

[2] A. Franquet et al., Vacuum 202 (2022) 111182

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Biomaterial Interfaces
Room 209 F W - Session BI1-MoM
Characterization of Biological and Biomaterials Surfaces

Moderators: Pierluigi Bilotto, TU Wien, **Morgan Hawker**, California State University, Fresno

8:15am **BI1-MoM-1 Determine Protein Conformation and Orientation at Buried Solid/Liquid Interfaces in Situ***, Zhan Chen,* University of Michigan **INVITED**

Interfacial protein properties play important roles in many research areas and practical applications, such as biomedical materials, marine antifouling coatings, membranes for biological molecule separation, biosensors using surface immobilized enzymes, and antibody drug manufacturing and storage, etc. The properties of proteins at interfaces are determined by molecular structures of interfacial protein molecules. In this study, a nonlinear optical laser spectroscopic technique, sum frequency generation (SFG) vibrational spectroscopy, has been used to determine conformations

[1] **ASSD Peter Sherwood Award**

and orientations of proteins at buried solid/liquid interfaces in situ in real time. A combined approach using molecular dynamics simulation, SFG experimental data, Hamiltonian spectra calculation, spectra matching, and isotope labeling was used for interfacial protein structure determination in this research. This method was successfully applied to study protein Gb1 adsorption to a variety of substrates, interfacial antibody – surfactant interactions, protein dimer formation at interface, membrane protein complex structure, and time-dependent protein structural change during the adsorption process.

8:45am **BI1-MoM-3 Cryo-XPS Characterisation and Solution Realism for Functional Nanoparticle Analysis**, ***Liam Soomary***, *Jonathan Counsell,* Kratos Analytical Limited, UK*; David Cant, William Lee,* National Physical Laboratory, UK

A crucial part of nanoparticle engineering relies on understanding and controlling surface functionalisation. Traditionally, analysis can be performed with techniques such as Transmission Electron Cryomicroscopy (CryoTEM) [1], however quantitative surface characterisation remains a challenging prospect.

X-ray Photoelectron Spectroscopy (XPS) has long been an exemplary technique for quantitative surface analysis, offering high sensitivity to elemental compositions and chemical states. However, its requirement for ultra-high vacuum (UHV) often compromises the relevant conditions under which most organic nanoparticle systems operate, leading to questions about their morphology and stability of their functionalised groups once the solvent environment is removed [2]. Recent developments in cryogenic XPS (Cryo-XPS) aims to bridge this gap. Through flash-freezing, liquid nanoparticles can be preserved in a close-to-native state within UHV conditions, minimising environment induced changes and enabling insights without significant structural perturbations [3].

In this talk, we discuss complementary techniques for solution-based measurements and highlight the benefits of Cryo-XPS in probing functionalised nanoparticles. Special attention is given to PEG-coated nanoparticles, which are widely used in drug delivery systems and biomaterials research. As we illustrate – through a case study of lipid nanoparticles – how sample preparation, handling and methodology can improve quantitative surface analysis of these systems.

[1] Judith Kuntsche *et al., Cryogenic transmission electron microscopy (cryo-TEM) for studying the morphology of colloidal drug delivery systems,* International Journal of Pharmaceutics, (2011), 120-137, DOI: 10.1016/j.ijpharm.2011.02.001
[2] S. Mourdikoudis *et al., Characterization techniques for nanoparticles: comparison and complementarity upon studying nanoparticle properties*, The Royal Society of Chemistry, (2018),12871-12934, DOI: 10.1039/C8NR02278J
[3] G. Weiseenberger *et al., Understanding the invisible hands of sample preparation for cryo-EM*, Nat. Methods, (2021) 18:5, DOI: 10.1038/s41592-021-01130-6

9:00am **BI1-MoM-4 GCIB-SIMS in the study of Lymphoma**, ***John Fletcher,*** *Simon Uzoni, Noora Neittaanmäki, Vasilis Chatzikyriako, Daniele Zanchin,* University of Gothenburg, Sweden

The advent of gas cluster ion beams (GCIBs) for SIMS has greatly benefited the analysis of biological samples through the generation of increased intact molecular secondary ions. This has enabled detailed molecular maps to be generated in order to perform "molecular pathology", elucidating chemical changes associated with different diseases. In this study GCIB-SIMS, in this case using a 40 keV $(CO_2)_{7k}^+$ ion beam on a J105 ToF-SIMS instrument (Ionoptika Ltd.) was used to map the intact lipid signals across 14 human lymph node samples representing diffuse large B-cell lymphoma (DLBCL) and control samples. DLBCL is a common and aggressive form of lymphoma resulting in a diffuse distribution of cancerous cells amongst the typical lymph cells. The analysis allowed the samples to be classified as malignant or non-malignant and also highlighted additional aggressive cancer signature in a DLBCL sample with an unusually high proliferation index. A complementary, combined k-means/image PCA approach was used to interrogate the data highlighting the pros and cons of the different approaches and potential sources for misclassification/diagnoses resulting from the heterogeneity of the DLBCL samples. Compared to other cancer samples the lipid markers associated with cancer can appear reversed as many studies have classed inflammatory responses to cancer as part of the cancer signature. In the lymph node tissue, the onset of malignant transformation is associated with a decrease in inflammatory character. While delivering new information regarding the chemistry of lymphoma the results also highlight the need for cellular precision with high chemical specificity and sensitivity, and the challenges associated with spectral/spatial classification of such complex samples and data where differently aggressive cancer samples show different signatures and pockets of different cell types, in this case histiocytes, can be show intermediate cancer/healthy lipid profiles.

9:15am **BI1-MoM-5 Optical Dynamics of Electrochemically Driven Reflectin Protein Films**, *Yin-Chen Lin, Dan Morse, Lior Sepunaru,* ***Michael Gordon,*** University of California at Santa Barbara

Near- and sub-wavelength photonic structures are used by different organisms (e.g., insects, cephalopods, fish, birds) to create vivid and often dynamically-tunable colors, as well as create, manipulate, or capture light for vision, communication, crypsis, photosynthesis, and defense. This talk will highlight our work to understand and translate the biological mechanism of reflectin, an intrinsically disordered protein found in squid skin cells that is responsible for dynamically tunable structural color, into new materials and device venues with the ultimate goal of using biological components and paradigms to create novel multi-scale structures with functional properties. Neuronally triggered-phosphorylation drives the condensation of reflectin proteins *in vivo*, resulting in osmotic dehydration of cell membrane-encapsulated layers of reflectin-loaded lamellae and low refractive index extracellular space that effectively function as a biological and tunable distributed Bragg reflector (DBR).

In close analogy to this physiological phenomenon, we demonstrate here that electrochemical reduction enables tunable and reversible control of reflectin condensation and thin film water fraction, allowing one to electrochemically tune reflectin film refractive index and thickness, just as that occurring in the squid [1]. Electrochemical correlative ellipsometry and surface plasmon resonance spectroscopy were developed to trigger and simultaneously analyze the dynamic changes in optical properties of reflectin films to further elucidate and mimic the color-changing mechanisms in squid skin. Measurements indicate that electrochemical reduction allows precise modulation of film refractive index (1.36 to 1.40) and thickness (40-100 nm). Condensation-driven, cyclical FRET emission from reflectin films is also demonstrated using electrochemical triggering as a preface to implementing reflectin as a triggerable optical medium in 1D gratings. Overall, this work opens new approaches to analyze biophysical mechanisms governing protein condensation and structural color regulation, and facilitates the design of bio-enabled functional materials and devices that bridge the biotic-abiotic gap.

[1] Y.-C. Lin, C. Yang, S. Tochikura, J.R. Uzarski, D.E. Morse, L. Sepunaru, and M.J. Gordon, Advanced Materials 2411005 (2025).

Biomaterial Interfaces
Room 209 F W - Session BI2-MoM
Biomolecules and Biophysics at Interfaces

Moderators: Kenan Fears, U.S. Naval Research Laboratory, **Markus Valtiner**, Vienna University of Technology, Austria

10:30am **BI2-MoM-10 How Swelling Affects Microscale Wetting and Friction of Soft Interfaces**, ***Jonathan Pham,*** University of Cincinnati **INVITED**

Soft materials are found in a host of applications, from adhesives and coatings to natural and synthetic biomaterials. Many of these materials comprise a lightly crosslinked polymer network, which can also be infused with a compatible liquid (i.e., swelling). Swelling offers additional functionality, like molecular transport, lubrication, and control over mechanical properties. However, understanding the behavior of soft and swollen interfaces is an ongoing challenge. For example, when crosslinked solids are sufficiently soft, or the characteristic size scale is small, they display liquid-like characteristics like capillarity, even without an infused liquid. When the networks are swollen, the swelling liquid itself provides true liquid behavior, creating multi-phase situations that are even more complex. Here we will leverage confocal microscopy to show how combinations of solid and liquid characteristics control the wetting on soft, swollen networks. In addition to network elasticity, we demonstrate that surface tension, liquid separation, and osmotic pressure are important considerations. We expand on our findings by developing a route to visualize dynamic contact lines of a dynamic, sliding drop. In addition to wetting, we exploit a combination of confocal microscopy and colloidal probe microscopy to study the effects of swelling on microscale friction. In this situation, creasing occurs, leading to solid-like stick-slip behavior.

Creasing is mitigated by swelling, which appears to be a function of the swelling ratios.

11:00am **BI2-MoM-12 Stability of Semi-Conducting Oxides Under Photocatalytic and Hydrogen Evolving Conditions**, *Tatjana Ott, Ruri Lee,* ***Markus Valtiner,*** Technische Universität Wien, Austria

Transparent semiconducting oxides play a critical role in fields ranging from corrosion, electrocatalysis and biocatalysis to the development of artificial leaf systems for solar fuel generation. However, their long-term stability remains a significant challenge, with photocorrosion being a major factor limiting performance. I will demonstrate how we employ an electrochemical flow cell coupled with inductively coupled plasma mass spectrometry (ICP-MS) to enable in situ, time-resolved monitoring of zinc release from zinc oxide (ZnO) single crystals under UV irradiation. This approach provides direct insights into the degradation pathways of ZnO, a key material in photoelectrochemical systems, including those inspired by natural photosynthesis.

We investigate the dissolution behavior of ZnO with (0001) and (10$\bar{1}$0) crystal orientations across a range of acidic and alkaline pH levels, examining potential-dependent dissolution under both oxygen and hydrogen evolution conditions. Our results highlight the significant influence of UV light and electrolyte pH on stability, closely linked to the intrinsic surface chemistry of ZnO. Notably, the polar ZnO(0001) orientation demonstrates superior stability at low potentials and under hydrogen evolution conditions. In contrast, non-polar ZnO(10$\bar{1}$0) exhibits higher dissolution rates, limiting its suitability for long-term water splitting and biocatalytic processes. It also highligths its role in corrosive processes where hydrogen can penetrate into materials leading to embrittlement.[1]

These findings underscore the critical role of surface structure and chemical stabilization in enhancing the durability of semiconducting oxides for materials stable against hydrogen permeation and next-generation energy conversion technologies. By optimizing surface design and understanding fundamental degradation mechanisms, it is possible to develop more resilient electroactive materials. I will discuss how the approach can be extended to other materials.

Reference.

[1] Dworschak et al. in ACS Appl Mater Interfaces, 2020 Nov 9;12(46):51530–51536. doi: 10.1021/acsami.0c15508 [https://doi.org/10.1021/acsami.0c15508]

[2] Ott et al. submitted

11:15am **BI2-MoM-13 PFAS-Protein Interactions: Effects of Perfluorooctanoate on the Structure and Function of Cytochrome C**, ***William Maza,*** US Naval Research Laboratory

The unique chemical nature of perfluoroalkyl substances (PFAS) renders it resistant to common metabolic processes. Consequently, the resulting bioaccumulation of FPAS has been implicated in long-term health risks associated with liver, kidney, and thyroid disease, increased cholesterol (hypertension and heart disease), disruption of reproductive function, and disruption of the immune response to name a few. However, the cytotoxic effects of PFAS in human organs is still poorly understood. Recent evidence points to increased levels of reactive oxygen species (ROS) as a primary source of cytotoxicity. The cause of the observed increase in ROS has to be established. To better understand the potential disruption of cellular respiration by PFAS we examine the effect of PFAS on the structure and function of the heme-containing electron carrier cytochrome c (Cc). We observe that in the presence of perfluorooctanoate (PFOA) Cc undergoes significant structural changes up to 2mM PFOA. These PFAS-induced conformational change include disruption of the putative MET80-heme charge transfer absorption band and increase in the Trp59 fluorescence indicating disruption of the Cc tertiary structure and at least partial exposure of the active site to water. The disruption of the heme coordination and tertiary structure of the Cc induces a significant change in the electrochemical redox potential of the active-site heme group which likely results in short circuiting its function as an electron shuttle between cyctochrome C reductase and cytochrome C oxidase in the electron transfer pathway. This likely results in downstream disruption of respiratory process and buildup of ROS.

11:30am **BI2-MoM-14 Confirmation of Jarzynski's Equality Based on Single Molecular and Macroscopic Interaction Force Measurements**, ***Iago Peters,*** *Markus Valtiner,* TU Wien, Austria

Knowledge about the free energy landscape of biomolecular reactions is necessary to understand how life works on the smallest scale. Unfortunately, obtaining experimental values of the free energy difference between two states like an unbound and a bound state of two molecules is rather difficult. [1] Jarzynski proposed an equality that connects the free energy difference between two states with the irreversible work that leads from one state to the other. Precisely, an average of all possible realizations of a process that moves the system from an equilibrium state to another state in equilibrium. Here, we test this hypothesis with experimental values. Using a simple model system, different nucleobase-pair interactions are measured using three different techniques that are able to measure the interactions force between two single molecules and up to 10^7 interactions in a single experiment run. Using the Atomic Force Microscope (AFM), Optical Tweezers and the Surface Force Apparatus allows us to additionally investigate the scaling of biological single molecule interactions. Together with molecular dynamics simulations a strong foundation is laid to confirm Jarzynski's equality and investigate the scaling of single-molecule interactions with a model system that is simplistic and biologically significant.

[1] 1. Gore J, Ritort F, Bustamante C. Bias and error in estimates of equilibrium free-energy differences from nonequilibrium measurements [Internet]. Vol. 100, Proceedings of the National Academy of Sciences. Proceedings of the National Academy of Sciences; 2003. p. 12564–9.

Corresponding/Presenting Author:Iago Peters, peters@iap.tuwien.ac.at

11:45am **BI2-MoM-15 Influence of Surface Structural and Electronic Properties on Antibacterial Action of Nano- and Microcrystalline Fe:ZnO**, ***Yuri M. Strzhemechny,*** *John H. Brannon, Dustin A. Johnson, Tiffany Y. McHenry, Devansh Kalluholematham,* Texas Christian University*; Rachel E. Cuth,* Kutztown University*; Kevin Srun,* James Martin High School

Antibacterial action of nano- and microcrystalline ZnO has been well established, although the fundamental mechanisms driving such cytotoxicity is still debated. In our recent works we suggested a model for an antibacterial action of ZnO via surface defect-mediated dissolution. To further validate our model, we perform surface/subsurface modification of hydrothermally grown ZnO nano- and microparticles in order to modulate their antibacterial efficacy. It appears that the instability of the ZnO in antibacterial assays results from the defect-rich reconstruction of polar surfaces with strong intrinsic dipole moment within the wurtzite lattice. In theory, Fe doping of ZnO may suppress this dipole and stabilize the free surface while preserving the wurtzite lattice. Importantly, iron ions are beneficial species for bacteria and thus do not change the cytotoxicity of the assay. We modify the hydrothermal synthesis protocol to obtain Fe:ZnO micro- and nanoparticles with controllable doping concentrations. We perform systematic optoelectronic and physicochemical characterization of our particles before and after their interaction with bacteria in different growth media to verify both the surface stability of our ZnO specimens and the effects on the antibacterial action.

12:00pm **BI2-MoM-16 Molecular Insights into the Influence of Tail Architecture on Self-Assembly of Peptide-Polymer Amphiphile**, ***Sabila Kader Pinky,*** North Carolina State University*; Benjamin Allen, Abigail Knight,* University of North Carolina at Chapel Hill*; Yaroslava Yingling,* North Carolina State University

Peptide-polymer amphiphiles (PPAs) combine functional peptides with a hydrophobic tail that drives self-assembly in aqueous environment. Their ability to form well-defined nanostructures with tunable physical properties makes them ideal candidates for a wide range of applications. However, predicting and tuning these features remains challenging due to the complex interplay of molecular interactions. Here, we systematically investigated the self-assembly of a random coil peptide (XTEN2)-based PPAs by varying the side chains of alkyl acrylate tail (ethyl, n-butyl, tert-butyl, hexyl, and cyclohexyl). We used all-atom molecular dynamics (AMD) simulations to examine how molecular interactions influence the formation, structure, and stability of micellar assemblies. The simulations reveal the formation of a range of core morphologies, including worm-like, perforated, spherical, and multi-core structures. Our findings indicate that the balance between tail-to-tail versus tail-to-water non-bonded interactions primarily determines the micellar morphology. Additionally, the extent of core hydration also impacts the structural stability. Furthermore, the comparison between experimentally obtained particle sizes and simulation-obtained particle sizes supports the accuracy of our computational approach in replicating real particle sizes and indicates that the models accurately capture the size characteristics of these self-assembled structures. We anticipate that the insight from this study will collectively provide a comprehensive understanding of how molecular properties and interactions drive the self-assembly and structural diversity of PPAs,

offering insights into designing nanostructures with tailored morphologies for specific applications.

Biomaterial Interfaces
Room 209 F W - Session BI1-MoA

Functional Biomaterials and Sensing

Moderators: Sapun Parekh, University of Texas at Austin, **Rong Yang**, Cornell University

1:30pm **BI1-MoA-1 Biodegradable Scaffolds Loaded with Metallic Particles for Enhanced Wound Healing**, ***Narayan Bhattarai***, NC A&T State University; *Alexis Moody, Sita Shrestha,* North Carolina A&T State University **INVITED**

Chronic wounds are a persistent clinical challenge, marked by impaired healing, infection susceptibility, and tissue degradation. To address these complexities, we developed bioactive nanocomposite scaffolds incorporating zinc (Zn) and magnesium (Mg) within the polymer polycaprolactone (PCL). Fabricated using electrospinning and 3D printing, these metal based scaffolds were designed to deliver soluble therapeutic ions while providing a structural framework to promote tissue regeneration.Due to their distinct biological roles, Zn and Mg were studied in scaffold formulations. In this study, Zn-loaded scaffolds improved fibroblast proliferation, collagen deposition, and cell differentiation. In vitro assays with NIH3T3 fibroblasts showed that Zn-containing scaffolds led to an increase in cell viability compared to controls and significantly enhanced migration and expression of α-SMA, vimentin, and collagen IV, key markers of fibroblast differentiation and matrix remodeling. Mg based scaffolds promoted cellular proliferation and supported anti-inflammatory effects, consistent with magnesium's role in modulating immune response and vascularization. Morphological analysis revealed that metal incorporation decreased fiber diameter, optimizing surface area and topography for cellular interaction, while ion release studies confirmed sustained Zn^{2+} or Mg^{2+} delivery under physiological conditions with minimal cytotoxicity. To further enhance scaffold performance, a subset of Zn scaffolds was surface-modified with a decellularized fibroblast-derived extracellular matrix (ECM), resulting in PZE scaffolds. This modification improved protein deposition, initial cell attachment, cell viability, and cell migration *in vitro*. *In vivo* studies in murine models demonstrated that the scaffolds supported tissue repair,showing early recruitment of M2-like reparative macrophages and improved healing responses compared to controls. These findings highlight the therapeutic potential of Zn and Mg as bioactive agents in wound healing applications. Their ability to provide targeted antimicrobial effects, modulate immune responses, and enhance tissue regeneration within tunable polymeric scaffolds presents a scalable, multifunctional strategy for treating chronic wounds. This approach holds promise not only for wound care but also for broader use in tissue engineering and regenerative medicine.

2:00pm **BI1-MoA-3 Molecular Modeling of Nucleic Acid-Based Nanomaterials**, *Elizabeth Skelly,* University of North Carolina at Charlotte; ***Christina Bayard***, North Carolina State University; *Joel Jarusek,* University of Nebraska; *Benjamin Clark,* North Carolina State University; *Laura Rebolledo, Yasmine Radwan, Phong Nguyen, Melanie Andrade-Muñoz,* University of North Carolina at Charlotte; *Thomas Deaton,* North Carolina State University; *Alexander Lushnikov,* University of Nebraska; *Sharonda LeBlanc,* North Carolina State University; *Alexey Krasnoslobodtsev,* University of Nebraska; *Yaroslava Yingling,* North Carolina State University; *Kirill Afonin,* University of North Carolina at Charlotte

DNA and RNA-based nanotechnology offers transformative potential for precision medicine, particularly in drug delivery and therapeutic applications, due to their inherent ability to precisely target and execute molecular functions. Nucleic Acid NanoParticles (NANPs) serve as versatile scaffolds for assembling functional nanomaterials. However, systematic understanding of how NANP design parameters, such as size, shape, sequence, composition, flexibility, and linker strands, govern their physicochemical properties and drive their self-assembly into supramolecular structures remains limited. Here, we employ multi-resolution molecular dynamics simulations, integrating all-atom (AA) and dissipative particle dynamics (DPD), to investigate how these parameters influence NANP structural, mechanical, and self-assembly characteristics. Furthermore, the integration of inorganic nanoparticles (NPs), such as quantum dots (QDs), into nucleic acid systems significantly enhances their functionality. QDs offer exceptional luminescence, photostability, and resistance to photobleaching, making them ideal biological markers. Functionalizing QDs with nucleic acids merges their superior optical properties with therapeutic functionalities. Due to the inherent limitations of experimental characterization techniques (e.g., TEM), we applied DPD simulations to elucidate mechanisms governing the formation and structural dynamics of QD-DNA condensates, providing detailed insights unattainable through experimental approaches alone. These findings advance our fundamental understanding of nucleic acid-based nanomaterials and facilitate their strategic development for next-generation biomedical applications.

2:15pm **BI1-MoA-4 Surface-Immobilized Fibronectin Conformation Drives Synovial Fluid Adsorption and Film Formation**, *Syeda Tajin Ahmed,* University of California Merced, United States Virgin Islands; *Ummay Honey, Lenka Vitkova, Diego Jaramillo Pinto, Katelyn Lunny, Warren Flores, Kaleb Cutter,* University of California Merced; *Yidan Wen, Kevin De France,* Queens University, Canada; ***Roberto Andresen Eguiluz***, University of California Merced

The articular cartilage extracellular matrix (ECM) is a complex network of biomolecules that includes fibronectin (FN). FN acts as an extracellular glue, controlling the assembly of other macromolecular constituents to the ECM. However, how FN participates in the binding and retention of synovial fluid components, the natural lubricant of articulated joints, to form a wear-protecting and lubricating film has not been established. This study reports on the role of FN and its molecular conformation in mediating macromolecular assembly of synovial fluid ad-layers. FN films as precursor films on functionalized surfaces, a model of FN's articular cartilage surface, adsorbed and retained different amounts of synovial fluid (SF). FN conformational changes were induced by depositing FN at pH 7 (extended state) or at pH 4 (unfolded state) on self-assembled monolayers on gold-coated quartz crystals, followed by adsorption of diluted SF (25%) onto FN precursor films. Mass density, thin film compliance, surface morphologies, and adsorbed FN films' secondary and tertiary structures reveal pH-induced differences. FN films deposited at pH 4 were thicker, more rigid, showed a more homogeneous morphology, and had altered α-helix and β-sheet content, compared to FN films deposited at pH 7. FN precursor films deposited at pH 7 adsorbed and retained more synovial fluid than those at pH 4, revealing the importance of FN conformation at the articular cartilage surface to bind and maintain a thin lubricating and wear protective layer of synovial fluid constituents. This knowledge will enable a better understanding of the molecular regulation of articular cartilage-SF interface homeostasis and joint pathophysiology and identify molecular interactions and synergies between the articular cartilage ECM and SF to reveal the complexity of joint biotribology.

2:30pm **BI1-MoA-5 Growable Mycelial Coatings: A New Approach to Bio-Based Plastic Replacements**, *Sandro Zier, Liza White,* ***Caitlin Howell***, University of Maine

Sustainable and compostable plastic replacements are in growing demand as we learn more about the health and environmental hazards associated with single-use plastic packaging. However, many biomaterials readily absorb water, making them unsuitable as plastic replacements, while hydrophobic bio-derived plastic alternatives can be expensive to produce. Here, we present an alternative: large-scale coating of a fungal mycelium mixture which grows exponentially over the course of three days to create a densely packed functional surface barrier. The resulting surface is highly hydrophobic (CA >130°) and absorbs water to the same degree as the current accepted standard for shipping materials (water uptake <30 g/m^2 after 120s). The grown coating also shows extremely high oil resistance and can withstand bending and folding. These findings highlight a promising path toward affordable, compostable, and high-performance biomaterials that address the pressing need for sustainable plastic alternatives while maintaining functionality for real-world applications.

2:45pm **BI1-MoA-6 Exploring New Materials as Biomimetic Growth Factor Delivery Systems**, ***Brooke Farrugia***, The University of Melbourne, Australia

Tissue engineering and regeneration is an inter-disciplinary field of research that combines principles from both biology and engineering. While the use of biomaterials has long been associated with this field of research, more recently there has been a paradigm shift for the modern biomaterial to be biomimetic, through replication of the *in vivo* situations they are trying to substitute. Growth factors and their use as a therapeutic is of great interest in tissue engineering and regenerative applications however, to achieve a beneficial response, appropriate administration of growth factors is required. Furthermore, due to biological heterogeneity of the molecules that control growth factor activity *in vivo*, their low abundance, and difficulty in isolation from mammalian tissues, there is a need to develop an alternative source of these biomimetic materials.

This prestation will explore the use of materials that mimic biologically derived sulphated sugar structures, known as glycosaminoglycans, that are responsible for the protection and delivery of growth factors *in vivo*. It was hypothesised that by adjusting structural variables, the specificity and affinity of these biomimetic materials towards different growth factors can be modulated, with the aim of developing a suite of materials that can be implemented in various tissue engineering applications to sequester and deliver growth factors and potentially modulate their downstream biological function.

3:00pm **BI1-MoA-7 Nanoparticle biosensing in 3D Cell culture**, *Miriam Kael, Paul Stoddart,* Swinburne University of Technology, Australia*;* ***Sally McArthur,*** Deakin University, Australia

While only a limited number of assays are tailored for 3D, and some are influenced by matrix proteins like collagen, nanoparticle-based biosensors present a valuable opportunity to analyse 3D in vitro cultures. Investigating how the sensor influences the model during in situ measurements is crucial, as is understanding how the model could interfere with the sensor's design. Certain sensors that exhibit potential in 2D may not be applicable in 3D environments. Although gold nanoparticles offer benefits, their detection in a 3D context is limited by traditional darkfield techniques. On the other hand, fluorescent nanodiamonds demonstrate significant potential as probes for 3D cultures.

Biomaterial Interfaces
Room 209 F W - Session BI2-MoA
Microbes and Biofilms

Moderators: Joe Baio, Oregon State University, **Caitlin Howell**, University of Maine

4:00pm **BI2-MoA-11 Influence of Copper on the Establishment of Marine Biofilms***, Sara Tuck,* ***Kenan Fears,*** U.S. Naval Research Laboratory

Biofouling, the accumulation of unwanted organisms on submerged assets, is an ongoing challenge within the maritime industry and has additional repercussions on human health. Biofouling build-up increases fuel consumption, asset drag, and operational costs in addition to facilitating the transfer of environmental and pathogenic bacteria from one location to another. Conventional methods to inhibit biofouling includes the application of antifouling coatings, the most popular of which are copper based. In biological systems, copper is tightly regulated and, in an attempt to exploit this, some antifouling coatings contain up to 75% copper (I) oxide by weight. Despite these high loadings, the efficacy of these coatings is rapidly declining with the emergence and spread of copper tolerant species. Microbial communities resistant to copper have been found to form mature biofilms on these coatings, which could be altering the interfacial properties to create more favorable conditions for the settlement of a broader biofouling community. To gain an understanding of the mechanisms responsible for the loss of antifouling performance, coated and uncoated polyvinyl chloride panels were deployed at field sites to harvest early biofilms. From these collections, we isolated, cultured, and identified bacterial species. Copper tolerance profiles were developed by re-exposing individual colonies to copper sulfate in broth microdilution assays. We also investigated copper biocide release from copper-ablative coated glass coverslips over a short time frame to better understand the copper environment that is susceptible to primary colonization.

4:15pm **BI2-MoA-12 Biofouling Prevention by Constant and Alternating Potentials***, Jana Schwarze, Emily Manderfeld,* ***Axel Rosenhahn,*** Ruhr University Bochum, Germany

The application of electrochemical potentials to surfaces is an easy and direct way to alter surface charge density, the structure of the electrochemical double layer, and the presence of electrochemically activated species. We investigated how applied potentials affect the colonization of surfaces by microorganisms. Different constant potentials as well as the regular alternation between two potentials were investigated, and their influence on the attachment of the biofilm-forming microorganisms on gold-coated working electrodes and laser induced graphene was quantified in laboratory and in field experiments. In order to be able to study the attachment under dynamic conditions, different electrochemical approaches have been developed to merge dynamic assay conditions e.g. microfluidics or rotating disks with potential control by potentiostats. In addition to the effect of the applied potentials on fouling, the electrochemical processes on the working electrode were analyzed by cyclic voltammetry and correlated with chemical analysis that provided insight into the reactive oxygen species formed. The electrochemical processes that occur on the surface will be discussed in view of the observed antifouling behavior and discussed regarding the protection of structures and ships in contact with seawater and technological applications such as desalination by reverse osmosis.

4:30pm **BI2-MoA-13 NO-Releasing Hybrid Material Coatings with Low Fouling Properties Against Pathogenic Bacteria***, Luciana Natascha Herbeck, Samantha Muhring-Salamone, Regina Kopecz, Axel Rosenhahn,* Ruhr-University Bochum, Germany

One serious, global issue facing human mankind is the uncontrolled accumulation and growth of organisms and organic matter onto man–made surfaces, known as biofouling.[1] Negative outcomes attributed to freshwater biofouling comprise clogging or corrosion, the spread of pathogenic bacteria in water distribution or food processing systems, and is the root of medicinal infections.[2–6] As the trend in coating design is moving towards sustainable and bio–friendly approaches, one strategy is to mimic nature's concepts in counteracting biofouling, e.g. by using secondary messenger molecules such as nitric oxide, which has been found to disperse biofilms and to exhibit antimicrobial effects.[7] This property has already been utilized in research on catheters and wound healing patches.[8,9] In this work, the secondary messenger molecule nitric oxide was integrated into a sustainable coating matrix consisting of the naturally occurring polysaccharide alginate, tetraethyl orthosilicate and an aminosilane capable to serve as an NO–acceptor/donor group. Two different nitrogen oxide species were formed in the coating after NO binding at elevated pressures and the ratio of the two species depended on the ratio of the two silane compounds. The NO-binding and release was characterized by UV-Vis spectroscopy and Griess–assays. Antifouling properties of the coatings against the freshwater bacteria *Bacillus subtilis*, *Pseudomonas fluorescens* and *Escherichia coli* were verified in dynamic attachment assays, revealing a significant reduction for NO–releasing samples compared to coatings without NO–release.

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Biomaterial Interfaces
Room Hall A - Session BI-TuA

The Future of Biointerface Science
Moderator: Tobias Weidner, Aarhus University, Denmark

2:15pm **BI-TuA-1 Quantifying Bacterial Adsorption at Biointerfaces Using Impedance Spectroscopy: A Key Step in Biofilm Formation***, Yunxing Li, Dipankar Koley,* Oregon State University

Bacterial adsorption is the first and important stage in the formation of biofilm on biointerfaces. A comprehensive understanding of this early stage of biofilm development helps us better control biofilm formation and evaluate the biointerfacical properties of various materials. To address the challenge of detecting subtle changes with this unstable bacterial adsorption in real time, here we developed a highly sensitive, flexible microsensor based on impedance spectroscopy to detect and quantify bacterial adsorption on different material surfaces using our innovative PEDOT coated electrode. These highly sensitive impedance electrodes gave a linear response to the amount of GFP-*E. coli*adsorbed. Furthermore, impedance-based methods enable monitoring of the kinetics of bacterial adsorption in real time. Utilizing this sensor, we observed stronger GFP-*E. coli* adhesion to positively charged glass than to regular glass. Additionally, we applied this sensor to metal ion-releasing resin composites to study how divalent metal ions (Zn^{2+}) control bacterial adsorption on these bioinerfaces. It not only allows for real-time quantification of bacterial adsorption, but more powerfully, it is capable of distinguishing between different material biointerface, which offers valuable potential for biointerface characterization.v

2:30pm **BI-TuA-2 Scalable and Biocompatible Polymer Dome Arrays for Oil-Free High-Resolution Live-Cell Imaging***, Kwang-Won Park, Sophie Liu, Wenjing Tang, Rong Yang,* Cornell University

High-resolution imaging of biological targets near the surface of glass coverslips conventionally requires immersion oil to match refractive indices and achieve optimal optical performance. However, this approach presents several limitations, including incompatibility with surface-sensitive cell types, potential cytotoxicity from oil infiltration into cell media, handling difficulties due to viscosity, and inapplicability with dry lenses. To address these challenges, we present a novel imaging platform based on polymer dome arrays (PDAs), nanoscale plano-convex polymer lenses fabricated via Condensed Droplet Polymerization (CDP), offering a scalable and biocompatible alternative to traditional oil-based systems. CDP enables rapid, vapor-phase production of PDAs with tunable sizes, radii of curvature, and surface densities directly on coverslips. The refractive index of the polymer material (n ~ 1.5) closely matches that of glass, eliminates immersion oil while enhancing diffraction-limited resolution. PDAs exhibited mechanical stability and optical precision during repeated imaging and confirmed biocompatibility with sensitive cell lines. To further enhance cell adhesion and minimize cytotoxic response, we applied conformal ultrathin polymer coatings atop the PDAs using initiated Chemical Vapor Deposition (iCVD) following CDP. These coatings significantly improved cell-substrate interactions while maintaining structural integrity and optical clarity over extended duration. This platform supports stable, long-term cell culture, allowing for real-time, high-resolution imaging at the single-cell level without reliance on immersion oil or advanced optical instrumentation. The combination of robust fabrication, superior biocompatibility, and optical performance positions this system as a versatile tool for live-cell imaging, mechanobiology, and high-throughput drug screening, where customizable, non-toxic substrates are essential.

2:45pm **BI-TuA-3 Development and Characterization of Decellularized Seaweed Scaffolds for Tissue Engineering.***, Gobinath Chithiravelu, Marion J. Jones, Ivana Hernandez de Estrada, Yadvendra Singh, Harish Subbaraman, Binata Joddar,* Oregon State University

In this study, the marine red seaweed *Devaleraea mollis* (commonly known as dulse) was investigated as a green, sustainable, and animal-free scaffold alternative, owing to its extracellular matrix (ECM) mimicking properties. A decellularization–recellularization approach was employed to develop cellulose-based scaffolds capable of supporting human cardiomyocyte growth. Native dulse samples were cleaned, dried, and decellularized using a combination of SDS (3, 5,7,10,12,15%), Triton X-100 (2%), and NaOCl (0.2%) in varying concentrations and time-dependent treatments. The resulting scaffolds were comprehensively characterized using light microscopy, scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), and Raman spectroscopy to identify the conditions that best preserved the fibrous, honeycombed architecture and cellulose-rich content of the native tissue. Among the treated scaffolds, those processed with 10%, 12%, and 15% SDS concentrations demonstrated the most favorable outcomes. These selected scaffolds were then subjected to swelling analysis to evaluate biodegradation behavior, followed by in vitro cell culture to assess biocompatibility all tested scaffolds demonstrated excellent compatibility with human cardiomyocytes, maintaining high cell viability over at least one week of in vitro culture, as confirmed by immunohistochemistry, quantitative cell analysis, and SEM imaging. Notably, SEM revealed over 50% surface coverage by cells on the scaffold by day six, indicating robust cell attachment and proliferation. Collectively, these findings highlight seaweed-derived cellulose as a highly promising, biocompatible, and eco-friendly biomaterial posing itself a novel interface for diverse biomedical applications, including scaffolds for cultivated meat production and innovations in sustainable tissue engineering.

Biomaterial Interfaces
Room Ballroom BC - Session BI-ThP
Biomaterial Interfaces Poster Session

BI-ThP-1 Antifouling Properties of Plastron Forming, Ultra-Porous, Superhydrophobic DCP- and PFPE-Based Coatings*, Georg Friedrich Breilmann,* *Louisa Vogler, Onur Özcan, Axel Rosenhahn,* Ruhr-University Bochum, Germany

One key problem of humanity for several thousand years has been biofouling. It occurs on artificial surfaces by creating biofilms consisting of organic matter, such as proteins, lipids or bacteria within seconds after immersion into seawater.[1,2] In addition, macrofoulers, e.g. algae or barnacles can attach and form slimy layers on the surfaces.[3,4] Biofouling has several detrimental consequences such as higher greenhouse gas emissions during propulsion, transfer of invasive species, and an increased work required to maintain immersed surfaces, all affecting both economy and environment.[5] To combat the formation of biofouling we created superhydrophobic surfaces (SHSs), which form a protective air layer between water and the submersed surface, so called plastrons. Five ultra-porous SHSs with different porosities, three based on ethylene glycol dicyclopentenyl ether methacrylateand two based on perfluoropolyether urethane methacrylate, were prepared by introducing porogens during the polymerization process. The coatings were tested regarding their superhydrophobicity, plastron formation, and plastron longevity. The wettability was analyzed by static and dynamic water contact angle goniometry to determine the wetting hysteresis as important quantities that characterize the ability of the terminating molecules of the coatings to reorientate once in contact with water. In addition, the water sliding angle was determined as an important property characterizing superhydrophobicity. Furthermore, the plastron forming and retaining properties of these SHSs were characterized by the visual plastron coverage, and the antifouling performance (AF) was tested in static attachment assays using the diatom *Navicula perminuta*. Additionally, the AF performance was investigated for fully functional plastrons, plastrons that were maintained for seven days by joule heating, and coatings on which the plastron decayed during this period.

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BI-ThP-2 Surface Sterilization by 260-280 nm Ultra-Violet C LEDs : Reducing the Probability of One Remaining Pathogen On A Surface to Less Than 10^{-6} – a Reproducibility & Accuracy*, Aarnav Sathish,* Arizona State University, SiO2 Innovates LLC, Arizona State University*; Nicole Herbots,* University of Missouri Kansas City, Arizona State University, University of California Santa Cruz*; Arjun Prabhu,* Arizona State University*; Anya Arun,* SiO2 Innovates LLC*; Zaid Abu-Salah,* University of Missouri Kansas City, SiO2 Innovates LLC*; Viraj Amin,* University of Missouri Kansas City, SiO2 Innovates LLC, Arizona State University*; Nachiket Rajinikanth,* University of Missouri Kansas City, SiO2 Innovates LLC*; Aditya Tyagi,* SiO2 Innovates LLC*; Yash Soni,* SiO2 Innovates LLC, Arizona State University*; Kush Patel,* SiO2 Innovates LLC, Arizona State University, University of California Santa Cruz*; Ashwin Suresh,* SiO2 Innovates LLC, Arizona State University, University of Arizona*; Shreyash Prakash,* SiO2 Innovates LLC, Arizona State University*; Nimith Gurijala,* SiO2 Innovates LLC, Arizona State University, Washington University in St. Louis*; Siddharth Jandhyala,* SiO2 Innovates LLC, Arizona State University, Duke University*; Arjun Sekar,* SiO2 Innovates LLC, Northwestern University*; Srivatsan Swaminathan,* SiO2 Innovates LLC, Arizona State University, Ichan School of Medicine at Mount Sinai*; Eric Culbertson,* SiO2 Innovates LLC*; Robert Culbertson,* Arizona State University

Antimicrobial resistance (AMR), hospital-acquired infections (HAI) and outbreaks are rising. 3M of AMR infections kill 50,000/y in the US and 1.3 M/ globally. AMR is projected to surpass cancer as the leading cause of death by 2050. Viral outbreaks now occur approximately every two years – twice as often as in the past 200 years: H1N1 (2009), MERS (2012), Ebola (2014), Zika (2015), and Covid (2019).

Effective surface sterilization must be rapid, reliable, safe, easy-to-deploy, and low-cost to address these issues. Sterilization, as defined by the US FDA, the EU and the International Standard Organization (ISO) is reducing the *'probability for a single viable microorganism to less than 10^{-6}*, a Sterility Assurance Level (SAL) of 6. Accepted methods (vaporized hydrogen peroxide (VHP), Ethylene Oxide(EtO), gamma irradiation (g), or autoclaving) cannot be used in public and hospital spaces, due to environmental, time, materials, and energy costs .

UVC irradiation eradicates pathogens by breaking bonds in nucleic acid pairs in DNA/RNA in water disinfection (SAL = 3) via 253.7 nm UVC fluorescent tubes. This work investigates whether low-cost low power LEDs can sterilize surfaces rapidly and reliably using *Lactobacillus Acidophilus.* (*Lacto. A*) as test pathogen and 260-280 nm UVC LEDs arrayed in a 4 cm^2 square with a power density of 0.8 ± 0.04 mW/cm^2 at 1 cm via two experiments, A and B. Two sets of *Lacto. A.* solutions are calibrated to a concentration of 1 x 10^7 and 2 x 10^7 Colony Forming Units (CFUs)/mL, and then serially diluted from 1.0 to 10^{-9}. In A and B, three sets of 10 agar plates are inoculated. The control set, 'No UVC' is compared to 2 irradiated sets, 'UVC1 and 2'. One half of the surface of each plate in UVC 1 and 2 is irradiated for 180 s, the other half left unirradiated.

Irradiation for 3 min yields an energy density of 144 ± 7 mJ/cm^2 on a 4 cm^2 square area with 2.5 x 10^5 CFUs/mL on the surface in A and 5 x 10^5 CFUs on the surface in B. In A, at a distance of 1.5 cm, 94 ±1 CFUs are left on the UVC1 culture set and 9 ± 3 CFUs on the UVC2 culture set. Thus, an average of 52 CFUs remain after UVC irradiation. This yields an SAL of 4. In B, at a distance of 1cm, UVC irradiation leaves an average of 7.5 CFUs remaining. This yields an SAL of 5. Therefore, UVC LEDs irradiation can consistently reach SALs above 3. The energy density at 1 cm needs to be increased by a factor of 10 to achieve sterilization with a SAL of 6, thus to 1.4 ± J/cm^2. This can be achieved by increasing the UVC LED power density to 8 mW/cm^2, or extending the duration of UVC exposure to 30 min.

BI-ThP-3 Dynamic Bonding (Dybonding) in DPD for Simulating DNA Hybridization and Self-Assembly*, Christina Bayard,* *Yaroslava Yingling,* North Carolina State University

Many problems modeled using Dissipative Particle Dynamics (DPD) require the ability to simulate chemical reactions, such as polymerization, cross-linking, DNA hybridization, and ligand-receptor binding, to accurately capture mesoscale phenomena in soft and biological materials. However, standard DPD force fields are inherently non-reactive, limiting their applicability to systems where bond formation or chemical specificity plays a critical role. In this work, DPD was utilized to explore how initial conditions influence the formation of Quantum Dot (QD)-DNA assembled condensates, a system driven by DNA hybridization between QDs functionalized with complementary strands. To address the computational challenge posed by modeling reactive behavior with inherently non-reactive force fields, we implemented an internally developed method called dynamic bonding (dyBonding), deployable within the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) simulation package. DyBonding enables selective, permanent bond formation based on distance and probabilistic rules between defined bead types. We further refined the approach to support directional, strand-specific bonding, allowing for complete DNA hybridization. This tailored approach offers a robust and efficient solution for modeling chemically reactive processes in DPD, expanding its applicability to a broader range of self-assembling and biofunctional systems. These novel methodologies substantially improve computational precision and expand the functionalities of widely used simulation packages such as LAMMPS. Enhanced understanding of nucleic acid interactions across multiple spatial and temporal scales enables the design of advanced materials for applications in drug delivery, therapeutics, and beyond.

BI-ThP-4 Plasma Diagnostics for the Modification of Naturally Derived Biopolymers*, Bethany Yashkus,* *Mollie Corbett, Joshua Blechle,* Wilkes University

Naturally derived biopolymers such as silk fibroin and chitosan show promise for use in biomedical devices due to their mechanical strength and slow degradation profile. Because these polymers are naturally hydrophobic, limitations in cell adhesion present challenges in applications that require short term degradation. To combat this, the surfaces of these materials are being altered using various inductively coupled plasma modification techniques. Surface analysis has shown that utilizing polymeric precursors with polar functionality, such as acrylic acid, can deposit a thin hydrophilic coating over the surface through plasma enhanced chemical vapor deposition (PECVD). Molecular precursors, such

as N_2, have also been used to alter hydrophilicity by introducing polar groups to the surface via plasma functionalization. In this work, acrylic acid treatments reduce the water contact angle (WCA) of silk fibroin from 75° to 47°, whereas nitrogen plasma treatments reduce WCAs from 75° to 40° for silk and 95° to 25° for chitosan.

To achieve a significant change in chitosan WCA, treating the sample for two minutes with a 25 mTorr, 115 W N_2 plasma containing 10% Ar has proven effective. In addition, when the films are casted on glass slides, the observed WCA of the glass is highly correlated with the WCA of the biopolymer.This suggests a synergy between the film and the underlying material. Due to these complex relationships, predicting ideal treatment conditions is not possible. Because little is known about the mechanisms that drive these surface modifications, optical emission spectroscopy (OES) is being employed to observe gas phase species during treatments and make diagnostic calculations such as species densities and vibrational temperatures. By cataloguing the trends in plasma species behavior with and without the presence of the biopolymer, key mechanistic contributors can be identified. Such insights allow for fine procedural adjustments, ultimately leading not only to desired surface outcomes but to reproducible plasma conditions.

BI-ThP-5 Effect of Surface Oxidation on Carbonic Anhydrase Immobilization on Graphene Oxide: A Molecular Dynamics Study, ***Merve Fedai**, Albert Kwansa, Youngwoo Hwang, Jialong Shen, Sonja Salmon, Yaroslava Yingling,* North Carolina State University

Carbonic anhydrase (CA) enzymes, which catalyze the conversion of carbon dioxide (CO_2) to bicarbonate (HCO_3^-), are promising candidates for improving the efficiency of existing carbon capture processes. However, their natural forms often lack the stability needed to maintain high activity over extended periods, especially under harsh industrial conditions. Immobilizing enzymes on surfaces is a widely used strategy to improve their durability and reusability. Experimental studies have shown that surface attachment can help overcome stability limitations, provided that catalytic activity is preserved. Graphene (GRA) and graphene oxide (GO) are effective matrices for enzyme immobilization due to their simplicity as model surfaces, electrical conductivity, and tunable surface chemistry. To examine the molecular-level interactions of this biomaterial system, all-atom molecular dynamics (AMD) simulations were performed. CA was modeled in contact with both GRA and GO surfaces to evaluate how surface chemistry affects enzyme structure and function. Various GO surfaces were constructed with oxidation levels ranging from 0% to 68% in 5% increments using a custom-built workflow for a systematic investigation of how surface oxidation modulates enzyme–surface interactions and potentially influences catalytic behavior. The simulations showed that oxidized GO surfaces form stronger hydrogen bonds and electrostatic interactions with CA, which help maintain the enzyme's structure, particularly near the active site. In contrast, GRA surfaces exhibit weaker binding, which may offer less stabilization but create fewer barriers to CO_2 diffusion. In addition to structural effects, the simulations revealed differences in CO_2 diffusion into the enzyme's active site. While GO enhances structural stability, stronger interactions may slightly restrict substrate access. GRA, on the other hand, allows faster diffusion but provides less structural support. Previous work with a different biomolecule suggested that GO oxidation levels between 15–25% yielded the best performance for biomaterial applications. However, due to the greater rigidity of CA, it remains uncertain whether the same range leads to optimal interaction and activity. These findings demonstrate that biomolecule-specific surface oxidation levels can be tuned to optimize enzyme performance.

BI-ThP-6 Macroscopic DNA/RNA Epi-Fluorescence (MaDRE) for Differentiated Detection of Bacterial, Viral and Fungal in Small Fluid Volume Diagnostic (Sfvd) Device: InnovaBugTM, ***David Guo**,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/College of Medicine, Drexel University/College of Medicine, University of Arizona*; Nithish Prakash,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC*; Sudharshini Ram, Arya Saravaran,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/BacteroBug LLC*; Nila Kathivaran,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC*; Sriram Rajesh,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/BacteroBug LLC*; Jonathan Guo,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC*; Robert Culbertson,* Department of Physics, Arizona State University*; Eric Culbertson,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/BacteroBug LLC*; Nicole Herbots,* Arizona State University/InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/BacteroBug LLC

The 21st century has seen 8 viral outbreaks, 5 due to new viruses. Better, faster, more accurate detection of viral infections is needed via low cost, fast, Small Fluid Volume Diagnostic (SFVD) devices that can be mass produced. Macroscopic DNA/RNA Epifluorescence (MaDRE) is here investigated to quickly and accurately detect viral infections and differentiate them from bacteria and fungi, before virus specific tests are available.

Detecting viral infections rapidly and reliably by differentiating viruses from bacteria and fungi can limit outbreaks where it is most needed in ER's, hospitals, and refugee camps.

In 2025, diagnostics for viral infections use Polymerase Chain Reaction (PCR) and virus-specific antigens but are not reliable. Covid-19 PCR swabs yield ~ 40% False Negatives (FN), ~ 50% False Positives (FP), and require 3 days and advanced labs to be performed. Covid Rapid Antigen tests yield 66% FNs and 40% FPs in asymptomatic individuals.

MaDRE is a new approach for detection of pathogens, via safe fluorescence microscopy stains inducing large scale fluorescence on 0.1 mL drops flattened into thin films. It is investigated here to prototype a new hand-held SFVD device, InnovaBug™, to detect and differentiate the 3 pathogen groups - bacteria, viruses, and fungi. This approach combines MaDRE stains, one specific to bacterial DNA, BacteroBug™, to viral RNA, ViroBug™, and to hydrophobins, FungiBug™, in drops of saliva, blood serum, urine, etc.

MaDRE in drops flattened into films is studied via calibrated pathogens solutions, using standard day-long plaque assays as controls. MaDRE's accuracy is measured by sampling four 0.1 mL drops of each solution. Reproducibility is measured by comparing MaDRE in 3 independent labs.

Strips are engineered to be tested within the same handheld analyzer, InnovaBug™, akin to a glucometer. For example, ViroBug™ test strips detect viral infections by combining 2 MaDRE stains and an RGB color analysis app.

Drops are applied on the test strip with 0.1 mL of a safe green and red DNA/RNA fluorophores, after lab-on-chip filters out blood and tissue cells. Blue light illuminates drops and yields red to green fluorescence ratio $R_{Red/Green}$ ($R_{R/G}$) in ≤ 30 min via the analyzer, and a smartphone for imaging and computing $R_{R/G}$. RRG detects viral loads ranging between 1 - 300 M Colony Forming Units/mL.

Results show MaDRE detects viruses quantitatively in 0.1 mL drops applied to ViroBug™ test strips, whose surface is engineered to be super-hydrophilic and can be analyzed in the InnovaBug™ SFVD analyzer. The InnovaBug™ analyzer prototypes and test strips are being optimized as small hand-held devices to be tested in triage situations.

BI-ThP-7 Differential Detection of Viral and Bacterial Infections by Macroscopic Epi-Fluorescence Combining DNA and RNA Specific Stains, *Nithish Prakash,* ***Sudharshini Ram**, David Guo,* Arizona State University / SiO2 Innovates LLC / InnovaBug LLC / Microbe Lab-On-Chip LLC*; Viraj Amin,* SiO2 Innovates LLC / Innovabug LLC / University of Missouri - Kansas City (School of Medicine) / Microbe Lab-On-Chip LLC*; Arya Saravanan, Sriram Rajesh, Nila Kathiravan,* Arizona State University / SiO2 Innovates LLC / InnovaBug LLC / Microbe Lab-On-Chip LLC*; Robert J. Culbertson,* Arizona State University*; Eric J. Culbertson,* SiO2 Innovates LLC / Microbe Lab-On-Chip LLC*; Nicole Herbots,* Arizona State University / SiO2 Innovates LLC / InnovaBug LLC

Six viral outbreaks in the last 15 years increased the need for viral detection at a triage level to contain these outbreaks. Standard viral diagnostics with rapid antigen testing yield ~58% False Negatives (FNs), and plaque assays take days to weeks for results. Annually, misdiagnosed infections cost hospitals $4.6 Billion, and antimicrobial resistance results in 35,000 deaths.

This work aims to reduce misdiagnoses to <10%, the gold standard, in detecting viral infections in 0.1mL of biofluids - blood, urine, etc. One fluorescent stain for bacterial DNA and one for viral RNA are combined to detect and distinguish bacterial and viral infections using Macroscopic DNA/RNA Epifluorescence (MaDRE). These stains were used with flattened drops on a *super hydrophilic* strip with ~1.5 mm diameter, 100 µm thin film, and surface area of ~1.8 cm^2, in order to prototype a low-cost, hand-held Small Blood Volume Diagnostic (SBVD) device, ViroBug™.

7 x 10^{10} Colony Forming Units (CFU)/mL of a benign virus, *T4 Bacteriophage*, are serially diluted into 10 solutions. 0.5 mL of each of the 10 dilutions (1.0, 10^{-1}, 10^{-2}...10^{-9}) is combined in a 1:1 ratio of undiluted 7 x 10^{10} CFUs/mL benign *E. Coli* bacteria host cells. As a control, each T4:*E. Coli* mix is tested via plaque assays. Six identical 0.1 mL drops of each T4 : *E. Coli* mix are applied onto test strips. 0.1 mL of safe green DNA-specific fluorescent dye is applied to the drops and photographed under 470 nm of blue light. Third, 0.1mL of safe red RNA-specific fluorescent dye is added to be fluoresced and imaged.

The ratio of green bacterial fluorescence (R_G) over blue illumination (R_B) and the ratio of red viral fluorescence (R_R) over green bacterial fluorescence (R_G) are calculated via a self-built app, FastRGB™. Raw ratios R_G/R_B and R_R/R_G are calibrated with background fluorescence to reduce photo-detector error, yielding R_{GNet} and R_{RNet}.

After analyzing 80 drops, R_{GNet} is 4.5 ± 0.3 with a relative error e of ± 7%. When T4 is diluted to 10^{-9}, R_{GNet} increases to 12 ± 2.6, with a bacterial load of 5 x 10^8 CFUs/mL with e of ±33%. Meanwhile, R_{RNet} decreases from 1.8 ± 0.2 for 5 x 10^8 CFUs/mL for 1.0 T4 Phage to 1.3 ± 0.06 for 50 CFUs/mL at 10^{-9} T4 Phage dilution.

R_{GNet} correlation with T4 load is 0.94 while R_{RNet} correlation is 0.96. Bacterial fluorescence (R_{GNet}), indicative of host cell survival, increases with decreasing viral load. Across 80 drops, 2 were identified as outliers, yielding an error rate of 2.5%. ViroBug™ produces rapid and accurate diagnoses using biofluid samples, fluorescent dyes, and automated color analysis.

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