## Biomaterial Interfaces
## Room West Hall - Session BI-TuA

### Future of Biointerface Science Collection (ALL-INVITED SESSION)

**Moderators: Kenan Fears**, U.S. Naval Research Laboratory, **Tobias Weidner**, Aarhus University, Denmark

2:45pm **BI-TuA-3 Adsorption of Cytochrome C on Different Self-Assembled Monolayers:the Role of Surface Chemistry and Charge Density**, ***Shengjiang Yang,*** School of Chinese Ethnic Medicine, Guizhou Minzu University, Key Laboratory of Guizhou Ethnic Medicine Resource Development and Utilization, China*; C. Peng,* School of Chemistry and Chemical Engineering, Guangdong Provincial Key Lab for Green Chemical Product Technology, South China University of Technology, China*; J. Liu,* Key Laboratory for Green Chemical Process of Ministry of Education, School of Chemical Engineering and Pharmacy, Wuhan Institute of Technology, China*; H. Yu, Z. Xu,* School of Chemistry and Chemical Engineering, Guangdong Provincial Key Lab for Green Chemical Product Technology, South China University of Technology, China*; Y. Xie,* Guangdong Provincial Key Laboratory of Electronic Functional Materials and Devices, Huizhou University, China*; J. Zhou,* School of Chemistry and Chemical Engineering, Guangdong Provincial Key Lab for Green Chemical Product Technology, South China University of Technology, China **INVITED**

Contradictory results regarding cytochrome c (Cyt-c) adsorption onto different self-assembled monolayers (SAMs) have been reported. In this work, the adsorption behavior of Cyt-c on five different SAMs (i.e., $CH_3$-SAM, OH-SAM, $NH_2$-SAM, COOH-SAM and $OSO_3^-$-SAM) were studied by combiningparallel tempering Monte Carlo and molecular dynamics simulations. The results show that Cyt-c binds to the $CH_3$-SAM through a hydrophobic patch (especially Ile81)and undergo a slight reorientation, while the adsorption on the OH-SAM is relatively weak.Cyt-c cannot stably bind to the 7% protonated $NH_2$-SAM even under a relatively high ionic strength condition, while a higher surface charge density (SCD, 25% protonated) promotes its adsorption. The preferred adsorption orientations of Cyt-c on the negatively charged surfaces are very similar, regardless of the surface chemistry and SCD. As the SCD increases, more counterions are attractedto the charged surfaces, forming distinct counterion layers.The secondary structure of Cyt-c is well-kept when adsorbed on all these SAMs.The deactivation of redox properties for Cyt-c adsorbed on the $CH_3$-SAM and highly negatively charged surface ($OSO_3^-$-SAM) is due to the confinement of heme reorientation and the farther position of the central iron to the surfaces.This work may provide insightful guidance for the design of Cyt-c-based bioelectronic devices and controlled enzyme immobilization.

3:00pm **BI-TuA-4 Spatiotemporal Control of Cellular Signaling Cues in 3D Biointerfaces for Tailored Cellular Functionality**, ***Sadegh Ghorbani,*** Stanford University*; D. Sutherland,* Aarhus University, Denmark **INVITED**

A promising research direction in the field of biological engineering is the development of programmable three-dimensional (3D) biointerfaces designed to support living cell functionality and growth in vitro, offering a route to precisely regulate cellular behaviors and phenotypes for addressing therapeutic challenges. While traditional two-dimensional (2D) biointerfaces have provided valuable insights, incorporating specific signaling cues into a 3D biointeractive microenvironment at the right locations and time is now recognized as crucial for accurately programming cellular decision-making and communication processes.The incorporation of advanced biomaterials, capable of responding to cellular cues and environmental changes, offers unique opportunities for creating these 3D environments. Emerging technologies, including nucleic acid nanotechnology (e.g., DNA origami, aptamers) and click chemistry, along with smart biomaterials, could further enhance the capabilities of these 3D biointerfaces. These tools allow for the submicrometer spatial organization of biomolecules over time, enabling the selective addition, removal, or shielding of signaling components through strand displacement or conformationally switched constructs. Leveraging these innovative tools also allows cell-membrane engineering, thereby enabling the precise organization of cells in appropriate spatial and temporal contexts to promote the formation of multicellular arrangements enhancing overall functionality. Developing cell-focused environments using 3D biointerfaces that deliver specific spatial and temporal signals can replicate complex biological functions into a finite set of growing cellular organizations. Additionally, they provide insights into the hierarchical logic governing the relationship between molecular components and higher-order multicellular functionality. The functional live cell-based microenvironment engineered through such innovative biointerfaces has the potential to be used as an in vitro model system for expanding our understanding of cellular behaviors or as a therapeutic habitat where cellular functions can be reprogrammed.

3:15pm **BI-TuA-5 Exploring the Dynamics of Proteins, Nucleic Acids, and Their Interplay by Coherent Anti-Stokes Raman Spectroscopy**, ***Pablo G. Argudo,*** *M. Brzezinski,* Max Planck Institute for Polymer Research, Germany*; W. Chen, B. Dúzs, A. Samanta, A. Walther,* Johannes Gutenberg University, Germany*; S. H. Parekh,* The University of Texas at Austin **INVITED**

The comprehension of proteins and nucleic acid chains, along with their interactions, is vital in contemporary biochemistry and molecular biology. These molecules can induce biological phase separation, resulting in the formation of membraneless organelles (MLOs) within cells. Consequently, understanding their structure is key, as it directly influence their ultimate behaviour. Moreover, external factors or interactions can directly impact their characteristics and final function, as evidenced in degenerative diseases like amyotrophic lateral sclerosis (ALS) or frontotemporal dementia (FTD).

In this context, we present the employment of Coherent Anti-Stokes Raman spectroscopy (CARS) as an appropriate method to characterize the changes happening over time in condensates. By examining the fingerprint region of nucleic acids, we can determine the biological interactions taking place. In designed DNA condensate model systems, ssDNA to dsDNA hybridization or salt effects can be monitored in the final assembled conformation. For proteins, their secondary structure can be elucidated, ranging from an ordered α-helix or β-sheet to a disordered random coil. Finally, protein-RNA interactions can be also characterized, as for TDP-43 low complexity domain (TDP43-LCD) and RNA. While introducing further complexity, the Raman shifts observed in specific regions of the formed condensates can indicate the RNA's effect on the protein, including secondary structure control.

# Author Index

## Bold page numbers indicate presenter