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Unraveling instructional cues for ordering the supramolecular structures of [redacted]

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Motivation

[redacted] represent a class of biomolecules that allow for controlled formation of ordered supramolecular networks—offering possibilities for biomedical and energy applications.[1–3] [redacted] hierarchical self-assembly into supramolecular structures through the synergistic effect of different intermolecular interactions.[4–6] However, due to the weak nature of the intermolecular interactions in [redacted] the resulting structures are often complex and dynamic. Characterization of these transient structures that contribute to the overall complexity [redacted] can be challenging; yet important towards understanding structure-dependent functionalities of the resulting materials.

In our research group, we currently design [redacted]. (Figure 1). [redacted] Photophysical characterization provide indirect evidence of their assembly, but for multicomponent systems, it is often challenging to determine the assembly features with high resolution. To fully realize the potential of these materials in devices, we will systematically explore the molecular design, fabrication parameters, and assembly triggers as instructional cues for [redacted]. Our *long-term goal* is to develop [redacted]

[redacted]

Figure 1. [redacted]

Project Description

In this project, we are *systematically exploring instructional cues that can be used to impart order on* [redacted]. In particular, we are designing the following [redacted]. We are committed to understanding the multi-scale structure-function relationships of the corresponding materials from these monomers. Due to the complexity and dynamic nature of the intermolecular interactions for these materials, elucidation of the hierarchical order adapted by the monomers require advanced characterization techniques such as *X-ray scattering, electron diffraction, micro-rheometry that are available through the state-of-the-art facilities in BioPACIFIC MIP*. Specifically, small-angle and wide-angle X-ray scattering (SAXS and WAXS) are important experimental characterization methods for studying the mesoscale ordered structures in soft materials. With a high intensity beamline such as the one in the BioPACIFIC MIP facility, we will be able to better elucidate the dynamic aspects of our material assembly. Moreover, microelectron diffraction (micro-ED) is useful to detect the crystalline molecular packing structures, especially for small nanostructures. Combining these characterization methods, the structural features from 0.1 to 100 nm scale can be detected. Furthermore, the micro-rheometer will be useful to reveal the mechanical properties of our hydrogel-forming peptides even with small sample volumes. With the above structural information, we will build a comprehensive

structure-function correspondence for our [redacted], thus, advancing the development [redacted].

Prior to performing experiments in BioPACIFIC MIP facilities, materials will be synthesized and their photophysical/electronic properties will be characterized in our laboratory. The following are our *specific objectives* for using the SAXS/WAXS, micro-ED, and micro-rheometer at BioPACIFIC MIP:

(1) Measure the X-ray scattering of functionalized [redacted] to obtain structural information in solutions, such as morphology, dimensional parameters, and density fluctuations (Quarter 1-2);
(2) Determine the molecular packing of functionalized [redacted] using micro-electron diffraction (Quarters 2-3);
(3) Measure the viscoelastic properties of [redacted] using the high-throughput micro-rheometer (Quarter 4);
(4) Correlate the structural and rheological properties of our [redacted] to the systematic variation in their molecular designs (*e.g.*, monomer sequence and length).

Desired Outcomes

(1) To elucidate the solution phase supramolecular structures formed by [redacted] through fitting the X-ray scattering data;
(2) To elucidate the molecular ordering of surface patterned [redacted] through analyzing the micro-electron diffraction data;
(3) To understand the structure-function relationship of these [redacted], from molecular structures, packing modes, mechanical properties, and optoelectronic properties;
(4) Based on the molecular structure- and instructional cue-dependent structure formation, we expect to gather insights about designing high-performance [redacted].

Broader Impacts and Synergies

The material characterizations that we will be able to perform at BioPACIFIC MIP will expand the current understanding of self-assembly processes in aqueous environments for our specific optoelectronic biomacromolecules. We are looking forward to including our findings, specifically on scattering/ diffraction/ rheology measurements, and new materials to the BioPACIFIC MIP libraries. In terms of synergies, our group is closely involved with the [redacted] which allows us to collaborate with other soft materials experts who may benefit from the results of this work and/or the knowledge of accessing BioPACIFIC MIP facilities. We are also open towards fostering other collaborations through the BioPACIFIC network, as well as to contribute to its diversity & inclusion goals—whether through outreach or sending out users who are researchers from underrepresented backgrounds. On this note, I should also mention that I am a co-organizer of [redacted] BioPACIFIC can be advertised during this event.

At this time, we request that the PI and 2 lab personnel [redacted]) from our research group be granted access to the Micro-ED, SAXS/WAXS, and high-throughput rheometer at the UCLA/UCSB BioPACIFIC MIP facilities.

References

[redacted]