University of California, Irvine THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING MSE 298 SEMINAR

FALL 2024: MSE IN THE SPOTLIGHT

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RESEARCH TALK:

SEQUENCE-PROGRAMMABLE ORDER-DISORDER TRANSITIONS IN SUPRAMOLECULAR PEPTIDE NANOFIBERS

DATE: Thursday, December 5, 2024 TIME: 2:00 - 3:00 PM LOCATION: McDonnell Douglas Engineering Auditorium Abstract: Hierarchical protein assemblies are governed by intricate chemical interactions that can be modulated by specific structural motifs and posttranslational modifications. This talk explores the dual impact of pHresponsive motifs and redox-sensitive disulfide staples on the secondary structure and assembly behavior of a designed coiled-coil peptide. The incorporation of adjacent lysine residues (KK) and strategically placed cysteine pairs enabled precise control over peptide conformation and nanofiber formation. We demonstrate that peptide sequences exhibit distinct structural transitions from random coil to β -sheet conformations in response to pH and oxidative conditions. Notably, oxidation-driven disulfide bond formation induced peptide cyclization, leading to the assembly of highaspect-ratio nanofibers with amyloid-like β -sheet architecture. Molecular dynamics simulations and kinetic studies highlight the critical role of sequence location, oligomerization, and the competitive interplay between intra- and inter-peptide disulfide bonding in determining assembly outcomes. The findings presented here offer insights into the design of stimuli-responsive peptide-based materials and provide a framework for understanding sequence-dependent pathways in amyloid fiber formation, with potential implications for neurodegenerative disease research.

Bio: Zack Urbach is a postdoctoral researcher in the lab of Prof. Allon Hochbaum investigating the hierarchical assembly and purification methods of peptide and protein nanostructures. He explores both bottom-up and topdown routes to isolate complex structures for the dynamic and functional manipulation of protein-based materials. Prior to UC Irvine, he obtained his PhD at Northwestern University under the direction of Prof. Chad Mirkin where we investigated the DNA-mediated and magnetic field directed assembly of iron oxide nanoparticles.