**Protein structure and dynamics in biomolecular condensates***Prof. Carlos R. Baiz*

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Cells achieve high spatiotemporal control over their biological processes through the compartmentalization of biomolecules either through membrane-encapsulated organelles or through the formation of biomolecular condensates (BMCs). These condensates consist primarily of proteins, and nucleic acids stabilized by strong electrostatic interactions as well as cation-pi, pi-stacking, and hydrogen bonding. Water makes up about 70% of the condensate volume, and water molecules are confined to nm-scale channels within the environment of the biomolecular condensate. Characterizing the dynamics of water and biomolecules within the condensate is essential for understanding the motions of biomolecules as well the interactions that lead to the structure, and phase stabilities. I will describe a combination of ultrafast two-dimensional infrared (2D IR) spectroscopy and molecular dynamics simulations to investigate the hydrogen-bond dynamics of model proteins and nucleic acids within the condensate phase. In addition, as part of our biocondensates characterization we seek to answer the question: “Do biocondensates promote folding?” We find residual secondary structure in otherwise disordered peptides. Further, we find that the mechanism of biocondensate formation (crowding vs. electrostatic) promotes different secondary structures.

As part of this seminar, I will introduce 2D IR spectroscopy and explain how the method can be used to probe protein structure and dynamics in complex systems. I will highlight a few examples from our lab. If time allows, I will describe new machine-learning approaches to improve signal-to-noise ratios using adversarial neural network techniques to reconstruct spectra from high-noise measurements. The machine learning methods are general and can be applied to many spectroscopic techniques across a range of optical implementations.