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Abstract for an Invited Paper for the MAR16 Meeting of the American Physical Society

## Tuning the entropic spring to dictate order and functionality in polymer conjugated peptide biomaterials SINAN KETEN, Northwestern University

Hybrid peptide-polymer conjugates have the potential to combine the advantages of natural proteins and synthetic polymers, resulting in biomaterials with improved stability, controlled assembly, and tailored functionalities. However, the effect of polymer conjugation on peptide structural organization and functionality, along with the behavior of polymers at the interface with biomolecules remain to be fully understood. This talk will summarize our recent efforts towards establishing a modeling framework to design entropic forces in helix-polymer conjugates and polymer-conjugated peptide nanotubes to achieve hierarchical self-assembling systems with predictable order. The first part of the talk will discuss how self-assembly principles found in biology, combined with polymer physics concepts can be used to create artificial membranes that mimic certain features of ion channels. Thermodynamics and kinetics aspects of self-assembly and how it governs the growth and stacking sequences of peptide nanotubes will be discussed, along with its implications for nanoscale transport. The second part of the talk will review advances related to modeling polymer conjugated coiled coils at relevant length and time scales. Atomistic simulations combined with sampling techniques will be presented to discuss the energy landscapes governing coiledcoil stability, revealing cascades of events governing disassembly. This will be followed by a discussion of mechanisms through which polymers can stabilize small proteins, such as shielding of solvents, and how specific peptide sequences can reciprocate by altering polymer conformations. Correlations between mechanical and thermal stability of peptides will be discussed. Finally, coarse-grained simulations will provide insight into how the location of polymer attachment changes entropic forces and higher-level organization in helix bundle assemblies. Our findings set the stage for a materials-by-design capability towards dictating complex topologies of polymer-peptide conjugate systems.