Ackert Hall, Room 120
Wednesday, August 27, 2025
4:00 P.M.

Coffee and Cookies
Chalmers Hall, Room 168
3:45 P.M.

Biochemistry & Molecular Biophysics Seminar

Sequence optimization of peptides that fold and self-assemble at water–solid interfaces

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Self-assembly is an efficient and inherently scalable route to constructing devices from single molecules; however, the major challenge is design of molecular components that form the desired structures with high fidelity. Polypeptides have many advantages as components of self-assembling functional materials, including physicochemical diversity, biocompatibility, well-understood structural motifs, and commercialized synthesis. Two-dimensional materials, such as graphene and hexagonal boron nitride, provide convenient substrates for assembly of molecular devices, owing to their atomically flat surfaces and electronic properties. Moreover, as compared to the fully 3D structures formed in solution, quasi-two-dimensional arrangements formed by peptides at solid–water interfaces facilitate imaging and human comprehension, as well as favoring more ordered peptide structures. Here, I will describe the computational design of cyclic peptides that fold and self-assemble at interfaces of 2D materials and experimental validation of these designs. Furthermore, using molecular dynamics simulation and free-energy calculation techniques, we have determined links between the peptide sequence and the thermodynamics and kinetics of folding and self-assembly. Specifically, we have found that glycine-threonine repeats best stabilize the folded β-sheet-like structure, while polyglycine or glycine-alanine repeats lead to stronger assembly. Turns with the glycine-proline-glycine-glycine sequence favor folding more than other tested sequences. These discoveries will help in future design of peptides that form programmable structures with high fidelity.