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Structural transformation of peptide amphiphile self-assembly induced by headgroup charge and size regulation CHANGRUI GAO, Northwestern University, MICHAEL BEDZYK, MONICA OLVERA, SUMIT KEWALRAMANI, Northwestern University, Materials Science and Engineering, LIAM PALMER, Northwestern University, Chemistry — The ability to control the nano and the meso-scale architecture of molecular assemblies is one of the major challenges in nanoscience. Significantly, structural transformations of amphiphilic aggregates induced by variations in environmental conditions have attracted attention due to their biotechnological relevance. Here, we study the assembly in aqueous solution for a modular series of peptide amphiphiles with 3, 2 or 1 lysine groups conjugated to a C_{16} carbon tail ($C_{16}K_3$, $C_{16}K_{2,}$ and $C_{16}K_1$). This system design allow us to probe how the equilibrium structure of the self-assembly can be tuned by controlling the coupling between steric (via choice of headgroup: K3, K2, or K1) and electrostatic (via solution pH) interactions. Solution small- and wide-angle X-ray scattering (SAXS/WAXS) and transmission electron microscopy (TEM) studies reveal that depending on pH and number of lysines in the lipid headgroup, amphiphiles can assemble into a range of structures: spherical micelles, bilayer ribbons and vesicles. We also perform detailed phase space mapping of pH-and headgroup size dependency of the structures of assembly over 0.1-100 nm length scales via SAXS/WAXS. The experimental results in conjunction with molecular dynamics (MD) simulations deduce quantitative relations between pH-dependent molecular charges, steric constraints and self-assembly morphologies, which is significant for developing experimental routes to obtain assembly structures with specific nano- and meso-scale features through controlled external stimuli.

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