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Self-assembled nanocages based on the coiled coil bundle motif NAIRITI SINHA, Department of Materials Science and Engineering, University of Delaware, JOSE VILLEGAS, JEFFERY SAVEN, Department of Chemistry, University of Pennsylvania, KRISTI KIICK, DARRIN POCHAN, Department of Materials Science and Engineering, University of Delaware — Computational design of coiled coil peptide bundles that undergo solution phase self-assembly presents a diverse toolbox for engineering new materials with tunable and pre-determined nanostructures that can have various end applications such as in drug delivery, biomineralization and electronics. Self-assembled cages are especially advantageous as the cage geometry provides three distinct functional sites: the interior, the exterior and the solvent-cage interface. In this poster, syntheses and characterization of a peptide cage based on computationally designed homotetrameric coiled coil bundles as building blocks is discussed. Techniques such as Transmission Electron Microscopy (TEM), Small-Angle Neutron Scattering (SANS) and Analytical Ultracentrifugation (AUC) are employed to characterize the size, shape and molecular weight of the self-assembled peptide cages under different pH and temperature conditions. Various self-assembly pathways such as dialysis and thermal quenching are shown to have a significant impact on the final structure of these peptides in solution. Comparison of results with the target cage design can be used to iteratively improve the peptide design and provide greater understanding of its interactions and folding.

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