Abstract Submitted
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Robust peptide bundles designed computationally[1] MICHAEL HAIDER, Univ of Delaware Materials Science and Engineering, HUIXI VIOLET ZHANG, Univ of Pennsylvania Department of Chemistry, KRISTI KIICK, Univ of Delaware Materials Science and Engineering, JEFFERY SAVEN, Univ of Pennsylvania Department of Chemistry, DARRIN POCHAN, Univ of Delaware Materials Science and Engineering — Peptides are ideal candidates for the design and controlled assembly of nanoscale materials due to their potential to assemble with atomistic precision as in biological systems. Unlike other work utilizing natural proteins and structural motifs, this effort is completely de novo in order to build arbitrary structures with desired size for the specific placement and separation of functional groups. We have successfully computationally designed soluble, coiled coil, peptide, tetramer bundles which are robust and stable. Using circular dichroism we demonstrated the thermal stability of these bundles as well as confirmed their alpha helical and coiled coil nature. The stability of these bundles arises from the computational design of the coiled coil interior core residues. The coiled coil tetramer was confirmed to be the dominant species by analytical ultra-centrifugation sedimentation studies. We also established how these bundles behave in solution using small angle neutron scattering. The form factor of the bundles is well represented by a cylinder model and their behavior at high concentrations is modeled using a structure factor for aggregates of the cylinders. All of these experiments support our claim that the designed coiled coil bundles were achieved in solution.

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