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Early Stages of De Novo Designed Beta-Hairpin Peptide Self-Assembly TUNA YUCEL, Department of Materials Science and Engineering, Delaware Biotechnology Institute, University of Delaware, Newark, DE 19716, JOEL P. SCHNEIDER, Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716, DARRIN J. POCHAN, Department of Materials Science and Engineering, Delaware Biotechnology Institute, University of Delaware, Newark, DE 19716 — In aqueous solution, MAX 1 peptide is unfolded and does not self-assemble. The peptide intramolecularly folds into a beta-hairpin when the electrostatic interactions between charged residues are screened through increasing the ionic strength at neutral pH. Beta-hairpin molecules supramolecularly assemble via hydrophobic collapse and hydrogen bonding into a 3-D hydrogel network. By combining the results of CD, cryo-TEM, DLS, and oscillatory rheology, we understand that the self-assembly proceeds by nucleation of monodisperse (3 nm wide) beta-sheet fibrils, which elongate, branch and cross-link to form clusters of fibrils. Assembly kinetics at this early stage indicates power law growth with assembly time. Eventually, clusters of fibrils interpenetrate to form a percolated network, as evidenced by the increasing network rigidity. The early stage assembly process will be discussed and compared to published gelation models.

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