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Self-assembly of Artificial Actin Filaments CHRISTOPHER GROSENICK, SHENGFENG CHENG, Virginia Polytechnic Institute and State University — Actin Filaments are long, double-helical biopolymers that make up the cytoskeleton along with microtubules and intermediate filaments. In order to further understand the self-assembly process of these biopolymers, a model to recreate actin filament geometry was developed. A monomer in the shape of a bent rod with vertical and lateral binding sites was designed to assemble into single or double helices. With Molecular Dynamics simulations, a variety of phases were observed to form by varying the strength of the binding sites. Ignoring lateral binding sites, we have found a narrow range of binding strengths that lead to long single helices via various growth pathways. When lateral binding strength is introduced, double helices begin to form. These double helices self-assemble into substantially more stable structures than their single helix counterparts. We have found double helices to form long filaments at about half the vertical binding strength of single helices. Surprisingly, we have found that triple helices occasionally form, indicating the importance of structural regulation in the self-assembly of biopolymers.

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