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Simulations and theory of model microtubule self-assembly[1] MARK STEVENS, SHENGFENG CHENG, Sandia National Labs, ANKUSH AGGARWAL, U. California at Los Angeles — We used molecular dynamics simulations to study the self-assembly of artificial microtubules. The model monomer has a wedge-shape to promote formation of rings that stack to form tubules. Attractive interaction sites are on the sides for ring formation and top/bottom for filament growth. We have studied the assembly kinetics and dynamics as a function of these lateral and vertical interaction strengths. A full structure diagram was calculated. The range of interaction strengths that best form tubules has been determined. We found that tubules form better when the lateral strength is stronger than the filamental stength, which contrast the picture for microtubules. The interaction strengths must be weak enough to allow for reformation of the clusters that initially form. Besides tubules, a variety of structures form depending on the interaction parameters. Interestingly, helical tubes and other helical structures are frequently observed despite the fact that the minimum energy substructure is a nonhelical ring. We have used a simple Flory-Huggins type theory to characterize the structure diagram.

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