Abstract Submitted
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Shape-designed single-polymer micelles: a proof-of-concept simulation[1] BRIAN MOTHS, THOMAS A. WITTEN, University of Chicago — Much effort has been directed towards self-assembling nanostructures. Strong, local interactions between specific building blocks often determine these structures (e.g., globular proteins). We seek to produce designed structures that are instead determined by collective effects of weak interactions (e.g., surfactant self-assembly). Such structures may reversibly change conformation or disassemble in response to changing solvent conditions, and, being soft, have potential to adapt to fluctuating or unknown application-imposed shape requirements. Concretely, we aim to realize such a structure in the form of a single polymer micelle—an amphiphilic polymer exhibiting a condensed, phase-segregated conformation when immersed in solvent. Connecting all amphiphiles into a single chain provides geometric constraints controlling the surface curvature profile, thus dictating a non-trivial shape. We present 2D Monte Carlo simulation results demonstrating the feasibility of such soft, shape-designed micelles. Preliminary results demonstrate a stable concave "dimple" in a micelle composed of a single A-B multiblock linear copolymer. We discuss both current limitations on shape robustness and effects of block asymmetry, block molecular weights and overall chain length on micelle shape.

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