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Computational Modeling of the Temperature-Induced Structural Changes of Tethered Poly(N-isopropylacrylamide)[1] JOHN G. CURRO, Sandia National Laboratories, SERGIO MENDEZ, Cornell University, JOHN D. MCCOY, NM Institute of Mining & Technology, GABRIEL P. LOPEZ, University of New Mexico — We modeled the effects of temperature, degree of polymerization, and surface coverage on the equilibrium structure of tethered Poly(N- isopropyl acrylamide) chains immersed in water. We employed a numerical self-consistent field theory where the experimental phase diagram was used as input to the theory. At low temperatures, the composition profiles are approximately parabolic and extend into the solvent. By contrast, at temperatures above the LCST of the bulk solution, the polymer profiles are collapsed near the surface. The layer thickness, and the effective monomer fraction within the layer, undergo what appears to be a first-order change at a temperature that depends on surface coverage and chain length. Our results suggest that as a result of the tethering constraint, the phase diagram becomes distorted relative to the bulk polymer solution and exhibits closed loop behavior.

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