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Atomistic Simulations of Poly(N-isopropylacrylamide) Surfactants in Water LAUREN J. ABBOTT, MARK J. STEVENS, Sandia National Laboratories — The amphiphilic polymer poly(N-isopropylacrylamide) (PNIPAM) displays a sharp phase transition at its LCST around 32 °C, which results from competing interactions of the hydrophobic and hydrophilic groups with water. This thermoresponsive behavior can be exploited in more complex architectures, such as block copolymers or surfactants, to provide responsive PNIPAM head groups. In these systems, however, changes to the hydrophobic/hydrophilic balance can alter the transition behavior. In this work, we perform atomistic simulations of PNIPAM-alkyl surfactants to study the temperature dependence of their structures. A single chain of the surfactant does not show temperature-responsive behavior. Instead, below and above the LCST of PNIPAM, the surfactant folds to bring the hydrophobic alkyl tail in contact with the PNIPAM backbone, shielding it from water. In addition to single chains, we explore the self-assembly of multiple surfactants into micelles and how the temperature-dependent behavior is changed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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