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Equilibrium and Kinetics of Block Copolymers Micelles JOSHUA MYSONA, DAVID MORSE, University of Minnesota — Both equilibrium properties of micelles, such as the critical micelle concentration (CMC), and dynamical properties such as the micelle lifetime are difficult to study in simulations because of the slow dynamics of the processes by which micelles are created and destroyed. We first discuss a method of precisely identifying the CMC in a simple model of block copolymer micelles in a homopolymer matrix, which makes use of thermodynamic integration to compute the free energy of formation. We then examine the free energy barriers to competing mechanisms for creating and destroying micelles, which could occur predominantly either by a step-wise process involving insertion and extraction of single molecules or by fission and fusion of entire micelles.

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