Abstract Submitted
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All-or-none folding of tethered polymer arrays[1] JOSEPH ROZALSKI, MARK TAYLOR, Hiram College — In this work we study the all-or-none folding transition of polymer chains tethered to a surface. This type of transition, similar to the folding transition of small proteins, provides a potential "on/off" switch to change surface properties and thus may be useful for smart-material and sensor device applications. We model the polymers as square-well-sphere chains and carry out Wang-Landau computer simulations. These simulations give the density of states, and thus the partition function, from which we can extract all thermodynamic information needed to study phase transitions. Here we investigate small arrays of chains of length N, end-tethered to a hard surface with tethering sites separated by distance Δx. For large enough Δx the chains undergo independent folding transitions, whereas, for small Δx the chains undergo a cooperative transition, co-folding into a single crystallite. This multi-chain transition involves a larger free-energy barrier than the single-chain transitions and thus has stronger "on/off" character. Effects of chain length, array size, and array geometry are also explored.

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Mark Taylor
Hiram College

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