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**Folding transitions of a multi-domain heteropolymer: A computer simulation study**[1] SU LATT, MARK TAYLOR, Dept. of Physics, Hiram College — Many biological macromolecules such as proteins and RNA fold into well-defined 3D conformations which are closely related to their function. Here we study folding transitions of a simple two-domain heteropolymer chain. The model chain consists of two alternating AB heteropolymers (A=square-well sphere, B=hard sphere), each consisting of N sites, linked by a section of M hard spheres. In this AB model the A-sites play the role of hydrophobic monomers while the B-sites act as hydrophilic monomers. We use Wang-Landau computer simulations to compute the density of states of this model polymer. From the density of states we construct the canonical partition function from which we can determine thermodynamic behavior. We have studied polymers with N = 16, 32, and 64 all with M = 10 for different square-well interaction ranges. With decreasing temperature the two AB domains undergo independent collapse transitions into on-average rod-like structures with the A-beads forming a linear core and the B-beads expelled to the surface. At very low temperatures these two collapsed rods combine to form a single rod with the linker expelled to the surface. In the future we hope to apply this type of model to both the folding of multi-domain proteins and protein-protein aggregation.

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