Abstract Submitted
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Phase diagram for 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 three-dimensional conformations that are closely related to their function. In this research, we study folding transitions of a simple two-domain heteropolymer chain. The model chain consists of two alternating AB sections (A=square-well sphere, B=hard sphere) linked by a section of B monomers. In this AB model, A-sites act as hydrophobic monomers and B-sites act as hydrophilic monomers. We use Wang-Landau computer simulations to compute the density of states of this model polymer, which allows us to construct the canonical partition function and single chain specific heat. We present a conformational phase diagram for the chain $(AB)_{32}(B)_{10}(AB)_{32}$ as a function of temperature and square-well interaction range. With decreasing temperature the AB-domains undergo simultaneous collapse transitions forming compact rod-like structures with an A-bead (hydrophobic) core and a B-bead (hydrophilic) exterior. There is evidence for a secondary transition in which the two collapsed AB domains join forming a single rod-like structure. For sufficiently long-range interactions there is also a low-temperature freezing transition in which the A-beads form a crystalline disk core with B-bead exterior.

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Mark Taylor
Dept. of Physics, Hiram College

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