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Folding transitions of a flexible/semi-flexible diblock or linked copolymer[1] CHRISTIAN WALKER, MARK TAYLOR, Dept. of Physics, Hiram College — Many chain macromolecules, such as proteins, undergo a folding transition into an ordered three-dimensional configuration for appropriate solvent conditions. In this research, we study the protein-like folding transition of the diblock copolymer. The model diblock copolymer is built by connecting two different chain segments, which each consist of Nseg square-well beads but have different bond lengths and thus different flexibilities (which is set by the bond length). We also study the effects of connecting the two identical domains via a semi-flexible hard-sphere linker consisting of Nlnk beads. We use Wang-Landau computer simulations to compute the density of states of this model and from this we construct the canonical partition function which gives all thermodynamic information about the system. Under the right conditions, we find that these diblock copolymers can undergo an all-or-none freezing transition in which the chains abruptly fold into compact structures with varying degrees of crystalline order depending on flexibility of the domains.

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