

Abstract Submitted
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Identification of transition from disordered to hexagonal ordered phase in simulations of asymmetric diblock copolymers PAVANI MEDAPURAM, DAVID MORSE, University of Minnesota — The transition from disordered to hexagonal ordered phase in asymmetric diblock copolymers has been identified precisely for a series of molecular weights using metadynamics which is a free-energy based technique. We explore important characteristics of the transition such as height of free energy barrier separating the two phases, first derivative of free energy, structure, strength of ordering, and compression modulus.

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