

Abstract Submitted
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Identifying the ODT in simulations of diblock copolymers using metadynamics JENS GLASER, DAVID MORSE, Dept. of Chemical Engineering and Materials Science, University of Minnesota — We propose a novel approach based on the structure factor as an order parameter and metadynamics as a free-energy technique to precisely locate the order-disorder transition in melts of symmetric diblock copolymers, which is fluctuation-induced first-order. We are able to directly measure the height of the free energy barrier separating the disordered and the ordered phase. We quantify finite size effects on the free energy minima and barrier.

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