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Quantitatively Accurate Simulations for Block Copolymer Melts (I)

Sunday 10 June 2018 12:00 (30 minutes)

Ideally, we would like to have first-principles simulations capable of quantitatively accurate predictions for any block copolymer system. Usually, our choice of model involves balancing the complexity needed to faithfully represent an actual experimental system and the simplicity required to make the simulation tractable. Fortunately, block copolymer phase behavior is believed to become universal in the high molecular-weight limit, which foregoes the need for detailed models. We illustrate how this universality can be used to make accurate predictions for a diblock copolymer melt from simulations using a simple lattice model. Nevertheless, simulations of blends and/or complex architectures are still extremely challenging even with the simplest of models. We conclude by discussing how this last obstacle could be overcome with field-theoretic simulations.

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