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Fluctuation Effects on Diblock Copolymer Melts using Field-Theoretic Simulations

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Self-consistent field theory (SCFT) has been remarkably successful in predicting the ordered phases of diblock copolymer melts. However, SCFT fails to predict the correct qualitative behavior along the order-disorder transition. It is well understood that this is because the saddle-point approximation of SCFT neglects fluctuation effects, which are particularly important for disordered phases. Here, we correct for this deficiency by performing field-theoretic simulations (FTS), where the field-theoretic Hamiltonian of SCFT is simulated. This brings the behaviour into full agreement with experiments. Most notably, the FTS provide the first confirmation that the complex Fddd phase is sufficiently stable to survive compositional fluctuations. As such, FTS appear to be a reliable means of accounting for the fluctuation effects neglected by SCFT. Furthermore, FTS can be easily generalized to more complex block copolymer systems, which is not the case for conventional particle-based simulations.

Primary author: Dr BEARDSLEY, Tom (University of Waterloo)

Co-author: Prof. MARK, Matsen (University of Waterloo)

Presenter: Dr BEARDSLEY, Tom (University of Waterloo)

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