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**Theoretically Informed Particle-Based Simulations of Polymers in Arbitrary Ensembles** DARIN PIKE, FRANCOIS DETCHEVERRY, University of Wisconsin, MARCUS MUELLER, University of Goettingen, JUAN DE PABLO, University of Wisconsin — A new, particle-based formalism is proposed for simulation of polymeric materials, where the interaction energy is given by the standard functional employed in field-theoretic models. The main features of the proposed formalism reside in its ability to enable simulations at constant stress or constant pressure, thereby permitting accurate estimation of free energies and phase boundaries. The usefulness of the proposed approach is illustrated in a series of thermodynamic property calculations from Monte Carlo simulations in the nVT, nPT, semi-grandcanonical and Gibbs ensembles. In particular, we consider the phase separation of a binary homopolymer blend and a symmetric diblock copolymer. For the blend, we present results for the phase diagram and the critical point of the model. For symmetric copolymers, we study the distribution of local stress in lamellae and the location of the first-order transition from a disordered to a lamellar phase.

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