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Recent advances in block copolymer mesoscale modeling: Numerical Self-Consistent Field Theory Simulations

SCOTT SIDES, NREL

Using block copolymers as mesoscale templates has potential applications for improved photovoltaic devices, fuel-cells and many others where the long-range order and orientation of the copolymer phase-separated domains is crucial. Self-consistent field theory (SCFT) for dense polymer melts has been highly successful in describing complex morphologies in block copolymers. Field-theoretic simulations based on SCFT theory are able to access large length and time scales that are difficult or impossible for particle-based simulations such as molecular dynamics. This talk will present recent results using PolySwift++, an object-oriented, high-performance framework for developing new SCFT algorithms. Included is an overview of a hybrid-SCFT algorithm for studying nanocomposites. This hybrid method allows simulations where the copolymer is treated within the field-theory framework, while the nanoparticle positions and orientations are included explicitly.