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Petascale Molecular Dynamics Simulations of Polymers and Liquid Crystals[1] TRUNG DAC NGUYEN, JAN-MICHAEL CARRILLO, W. MICHAEL BROWN, Oak Ridge National Laboratory — The availability of faster and larger supercomputers and more efficient parallel algorithms now enable us to perform unprecedented simulations approaching experimental scales. Here we present two examples of our latest large-scale molecular dynamics simulations using the Titan supercomputer in the Oak Ridge Leadership Computing Facility (OLCF). In the first study, we address the rupture origin of liquid crystal thin films wetting a solid substrate. Our simulations show the key signatures of spinodal instability in isotropic and nematic films on top of thermal nucleation. Importantly, we found evidence of a common rupture mechanism independent of initial thickness and LC orientational ordering. In the second study, we used coarse-grained molecular dynamics to simulate the thermal annealing of poly(3-hexylthiophene) (P3HT) and Phenyl-C61-butyric acid methyl ester (PCBM) blends in the presence of a silicon substrate found in organic solar cells. Our simulations show different phase segregated morphologies dependent on the P3HT chain length and PCBM volume fraction in the blend. Furthermore, the ternary blend of short and long P3HT chains with PCBM affects the vertical phase segregation of PCBM decreasing its concentration in the vicinity of the substrate.

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