

Abstract Submitted
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Molecular Theory Studies of Polymer/Nanoparticle Blends Near Surfaces¹ ERIN MCGARRITY, Dept. of Chemical Engineering & Materials Science, Michigan State University, AMALIE FRISCHKNECHT, Computational Materials Science & Engineering, Sandia National Laboratories, MICHAEL MACKAY, Dept. of Chemical Engineering & Materials Science, Michigan State University — Recent experimental results have shown that nanoparticles added to supported thin polymer films can inhibit dewetting by migrating to the substrate. To better understand this phenomenon, we use a classical density functional theory developed by Tripathi and Chapman. The effects of nanoparticle radius and density are examined. Preliminary results for hard-particle hard-chain systems indicate that regular layered structures emerge when a critical density is reached and the particles displace the polymers near the substrate. The effects of particle and polymer attractions and substrate potentials are currently being studied. We also compare our results to molecular simulations.

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