

4CF13-2013-000188

Abstract for an Invited Paper
for the 4CF13 Meeting of
the American Physical Society

Theory and simulations linking molecular features to morphology in polymer nanocomposites

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To engineer polymer nanocomposites for target macroscopic properties, it is important to find ways to control the spatial arrangement of nanoscale additives within the polymer matrix. In this talk, I will present our recent theory and simulation work focused on linking molecular features of the additives and polymers to the morphology of the composite. Two specific studies will be discussed. First, I will show how polydispersity in homopolymers grafted on the nanoadditives stabilizes dispersed morphology of the additives in the nanocomposite. Second, I will show how polymer architecture and additive-polymer miscibility affect morphological features, such as interfacial area and domain shapes, in conjugated polymer based composites.