Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Field-theoretic simulations of polymer nanocomposites containing grafted nanoparticles ROBERT RIGGLEMAN, HUIKUAN CHAO, JASON KOSKI, University of Pennsylvania — As polymer nanocomposite materials have found their way into an ever-growing number of applications, it has become clear that the dispersion state of the nanoparticles can play a key role in the resulting material properties. In some instances, it is ideal to have well-dispersed nanoparticles in a polymer matrix to facilitate high loading, while in other cases, self-assembled structures are preferred. A common route for controlling the dispersion state of the nanoparticles is to graft the particles with polymer chains, and efficient computational methods capable of predicting the limits of dispersion, aggregation, and the structure of any self-assembled particles could go a long way towards enabling the design of future polymer nanocomposite devices. To that end, we have extended the field-theoretic simulations framework to include grafted nanoparticles, where polymer chains can be grafted to the surface of hard nanoparticles. Our method is compatible with both self-consistent field theory and fully-fluctuating field theoretic simulations. Calculations will be shown for the distribution of grafted nanoparticles in homopolymer thin films as well as binary homopolymer blends, where our results agree very well with recent experiments.

Robert Riggleman
University of Pennsylvania

Date submitted: 16 Nov 2013 Electronic form version 1.4