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Viscoelastic Properties of Model Polymer Nanocomposites JAMES THOMIN, SUCHIRA SEN, PAWEL KEBLINSKI, SANAT KUMAR, Rensselaer Polytechnic Institute — The study of the dynamics of polymers in the presence of nano-scale particles is not only of fundamental interest but is also key to developing the tools necessary to engineer polymer nanocomposite materials. In this work, we investigate the effect of nanoscopic filler particles on the viscoelastic behavior of a model polymer melt. Molecular Dynamics simulations of bead-spring polymer systems containing roughly spherical nano-filler particles were performed. Equilibrium and non-equilibrium methods were used to determine the stress relaxation and shear-dependent viscosity of both the neat melt and filled systems. We will discuss the results of these simulations, as well as an interesting correlation between certain structural quantities and the observed mechanical reinforcement.

> James Thomin Rensselaer Polytechnic Institute

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