

Abstract Submitted  
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**Structure formation in nanocomposite hydrogels** DILIP GERSAPPE, DI XU, Stony Brook University — We use Molecular Dynamics simulations to study structure formation in physically associating nanocomposite hydrogels. Nanofillers were modeled as rigid bodies of disk-like shapes and physical crosslinks were simulated by introducing a short-range attraction between the nanofillers and polymer chain ends. The structure, dynamics and mechanics of this polymer gel was studied as function of nanofiller volume fraction. We observe the formation of a percolated network of these structures, with an ordered local structure but disordered globally, as we increase the filler fraction. The dynamics of polymers showed significant caging effects in the gel state. Stress autocorrelation and elongation results were analyzed as a function of the nano-filler concentration.

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