

Abstract Submitted
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A Novel Approach for Understanding the Effect of Nano-Fillers on the Conformational Properties of a Polymer Matrix: Dimensions go up or down? FATIH M. ERGUNEY, WAYNE L. MATTICE, The University of Akron — MC simulations of a polymer matrix composed of linear POE chains and nano-fillers were performed on a 2nd lattice to reveal the change in the $\langle s^2 \rangle$ of matrix chains perturbed by nano fillers. Nano-fillers are obtained by the collapse of a desired number of linear chains by increasing the contribution of the attractive core of discretized intramolecular LJ potential. The resulting change in $\langle s^2 \rangle_{matrix}$ is case sensitive in such a way that it might either go up or down depending on the size of both species. It tends to increase in the presence of nano-fillers when both kinds are represented by a small number of beads. There's a peak point observed in this case after which the dimensions start to decrease as the filler fraction is further increased. The contraction of chains is also of concern provided that chains have a larger number of beads. On the contrary, there's no peak point observed in such a case, but a plateau region is acquired at high filler fraction. Magnitude of the change depends on several parameters like mobility and compactness of fillers.

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