Supporting Information

A novel shift in the glass transition temperature of polymer nanocomposites: A molecular dynamics simulation study

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1. Diffusion of NP in polymer solution

We have simulated a single NP diffusion in polymer solution. In the system of size 40×40×40, we put 44 polymer chains of length 64. Here size of NP is $\sigma_{NP} = 1$. The density of polymer monomers is about 4.4%. The interactions between NP and polymer and between polymer and polymer are purely repulsive for simplification. NVT simulations are performed at temperature $T = 1$. The results of mean square displacement (MSD) of NP at different time (t) is present in **Figure S1** for NP of mass 1 and 100. We find the diffusion of NPs decreases with increasing NP's mass.

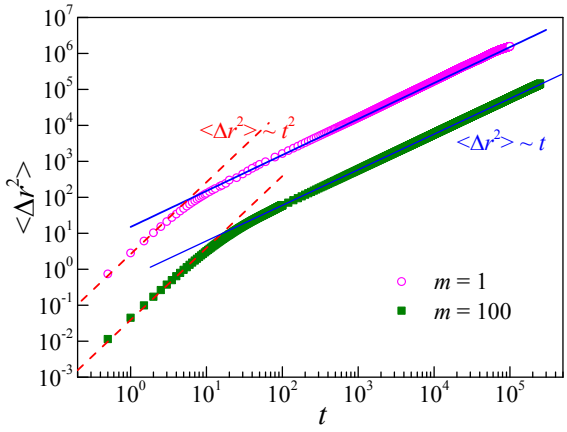

Figure S1. Plot of the mean square displacement of the NPs as a function of time for single NP in polymer solution at temperature $T = 1$.

2. Dependence of T_g on polymer chain length

We have checked the dependence of T_g on the polymer chain length for the pure polymer system. The result of the influence of polymer chain length on T_g is plotted in **Figure S2**. During the simulations, the number of polymer chains, $n = 44$, is fixed while the length of the polymer chain, N, is varied from 34 to 114. We find T_g increases with polymer length, in agreement with experimental results.[1] The polymer length dependence of T_g can be well fitted to the empirical Fox-Flory equation[2]

$$T_g(N) = T_g^{\infty} - \frac{C}{N} \quad . \tag{1}$$

We estimate $T_g^{\infty} = 0.525$ for infinitely long polymer chain.

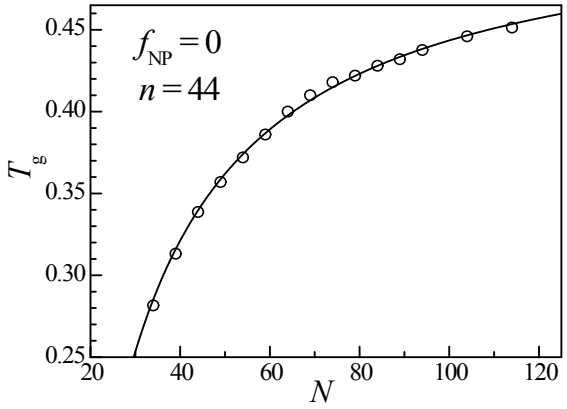

Figure S2. Simulation results for the variation of T_g with chain length N for the pure polymer system ($f_{NP} = 0$) with the number of polymer chains $n = 44$. The solid line is the best fit by the

empirical Fox-Flory equation (Eq. 1).

References:

[1] J. Hintermeyer, A. Herrmann, R. Kahlau, C. Goiceanu and E. Rossler, *Macromolecules*, 2008, **41**, 9335–9344.

[2] J.-L. Barrat, J. Baschnagel and A. Lyulin, *Soft Matt*., 2010, **6**, 3430–3446.