Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

Role of nanoparticle network in polymer mechanical reinforcement: Insights from molecular dynamics simulations

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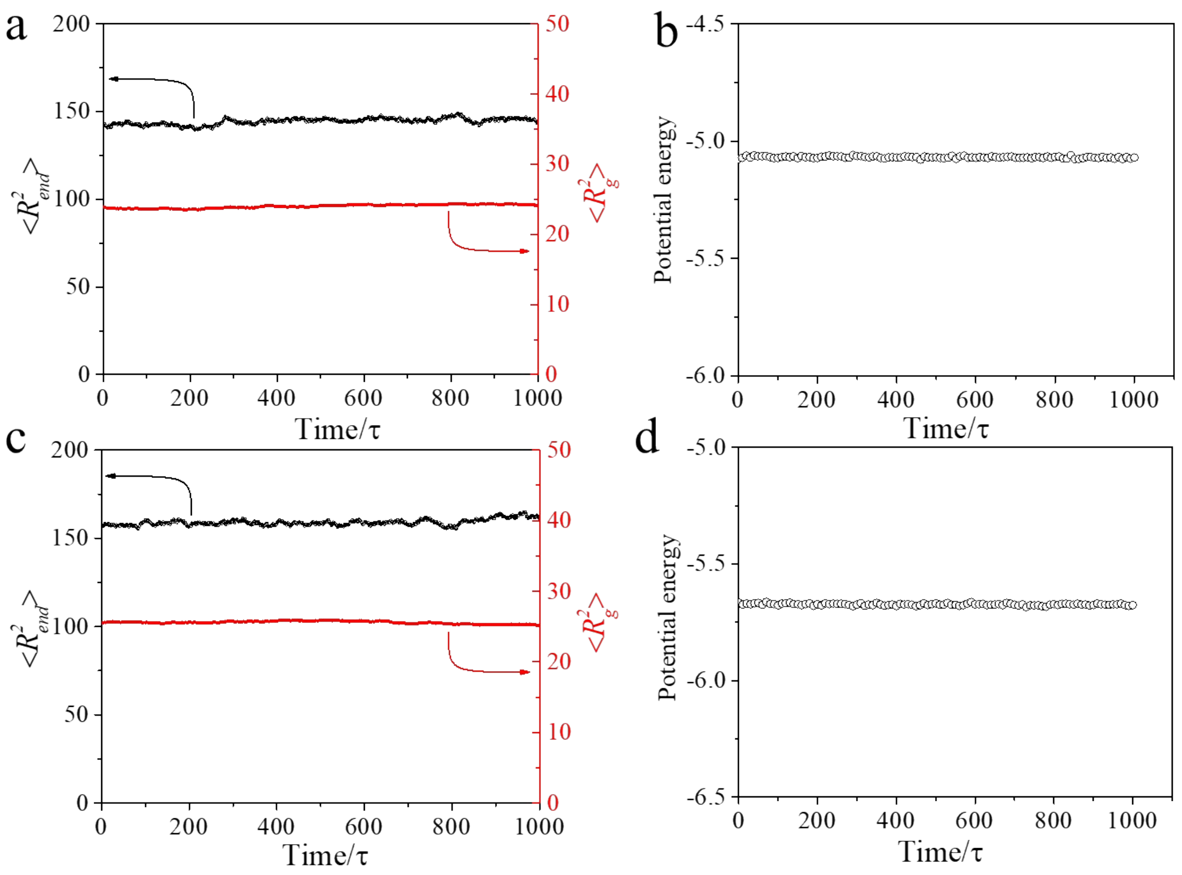

Fig. S1. (a, c) The variation of mean squared end-to-end distance R^2_{end}, radius of gyration R^2_g and (b, d) the change of the potential energy of the two systems in the following 1.0×10^6 MD steps after enough equilibration with *NVT* ensemble. For a and b, the NP-polymer interaction strength ε_{np} equals 2.0, NP-NP interaction strength ε_{nn} equals 20.0, and r_{cutoff} equals 2.5. For c and d, the NP-polymer interaction strength ε_{np} equals 2.0, NP-NP interaction strength ε_{nn} equals 50.0, and r_{cutoff} equals 2.5.

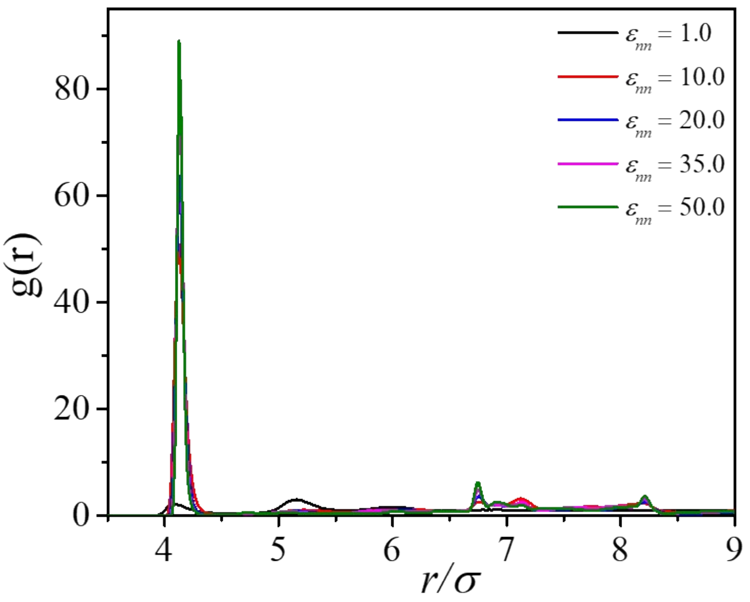

Fig. S2. Radial distribution function (RDF) of NPs for systems with different NP-NP interactions ε_{nn}. Note that the NP-polymer interaction strength ε_{np} equals 2.0, r_{cutoff} equals 2.5.

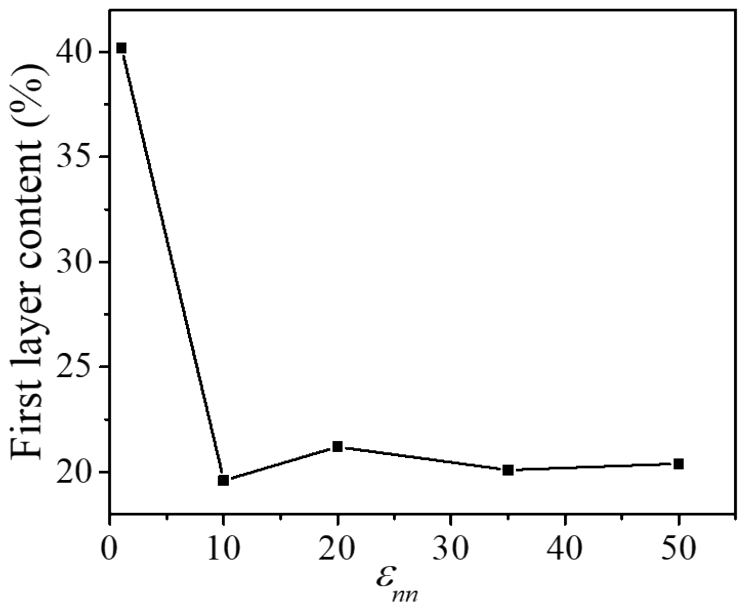

Fig. S3. Plot of the first layer content with respect to the NP-NP interactions ε_{nn}. Note that the NP-polymer interaction strength ε_{np} equals 2.0, r_{cutoff} equals 2.5.

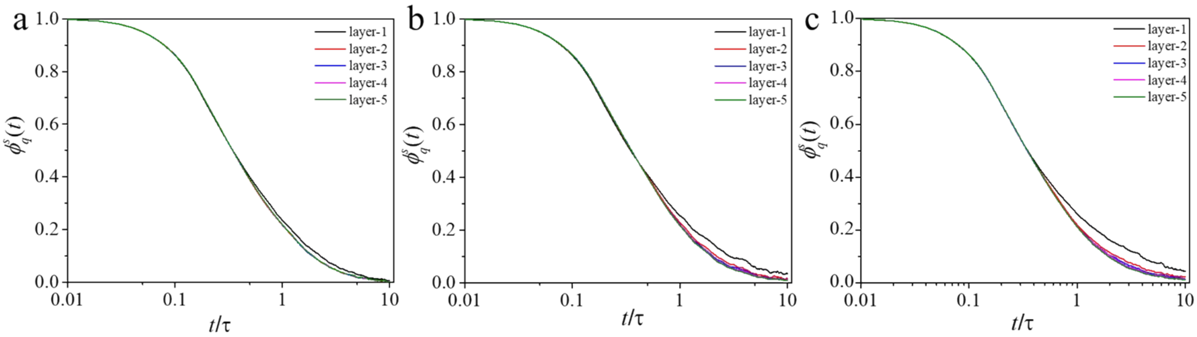

Fig. S4. Incoherent intermediate dynamic structure functions ($\phi_q^s(t)$) for the different polymer layer (from layer 1 to layer 5) around NPs in PNCs with different NP-NP interactions ε_{nn} at the segment length scale. (a) $\varepsilon_{nn} = 1.0$. (b) $\varepsilon_{nn} = 20.0$. (c) $\varepsilon_{nn} = 50.0$. The thickness of each polymer layer is unified as 1 σ. Note that the NP-polymer interaction strength ε_{np} equals 2.0, r_{cutoff} equals 2.5.

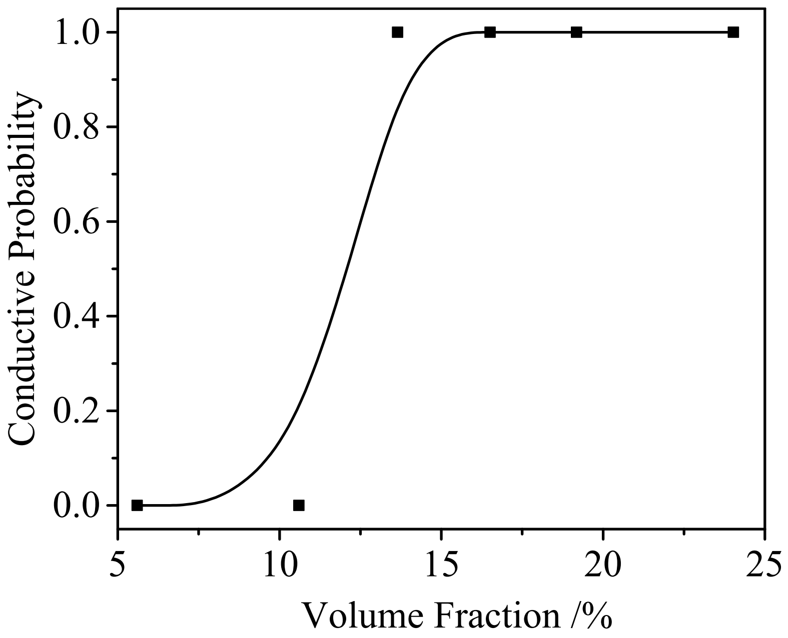

Fig. S5. The conductive probability of the nanocomposites at various volume fraction. Note that the NP-polymer interaction strength ε_{np} equals to 2.0, NP-NP interaction strength ε_{nn} equals 50.0, and r_{cutoff} equals 2.5.

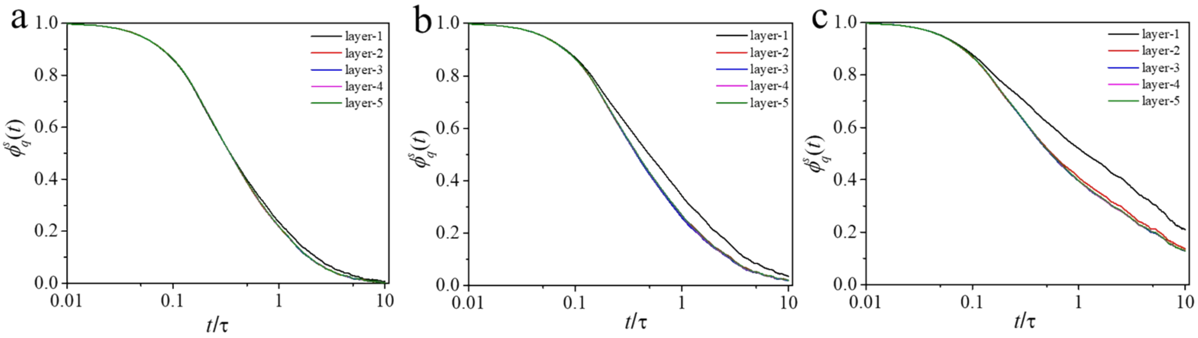

Fig. S6. Incoherent intermediate dynamic structure functions ($\phi_q^s(t)$) for the different polymer layer (from layer 1 to layer 5) around NPs in PNCs with different NP-polymer interactions ε_{np} at the segment length scale. (a) ε_{np} = 2.0. (b) ε_{np} = 5.0. (c) ε_{np} = 8.0. The thickness of each polymer layer is unified as 1 σ. Note that the NP-NP interaction strength ε_{nn} equals 1.0, r_{cutoff} equals 2.5.