Supplementary Information

Elucidating and tuning the strain-induced non-linear behavior of polymer nanocomposites: a detailed molecular dynamics simulation study

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Figure S1. Schematic of the Lees-Edwards "sliding brick" boundary conditions.

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Figure S2. Plots of specific volume versus temperature for the chain length N=30. The abrupt changes in the specific volume in Figure S2(a) and S2(b) are considered as a classical signature of the glass transition and the flow zone for a polymer, respectively.



Figure S3. The elastic modulus versus the tensile strain for neat polymer with different chain lengths



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Figure S4. (a) The snapshots of the designated system with six aggregates being uniformly distributed in the polymer matrix. The spheres with different colors denote separate NP aggregates, and the blue points denote the polymer chains. (b) the modulus strain curves of this designated system. (c) the number of neighboring NPs directly contacting with each other during the deformation process.

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Figure S5. The elastic modulus of the good dispersion system compared with the poor dispersion system. The tensile strain rate is set as 0.00327/τ.