Effect of shape and size of nanofillers on the viscoelasticity of polymer nanocomposites

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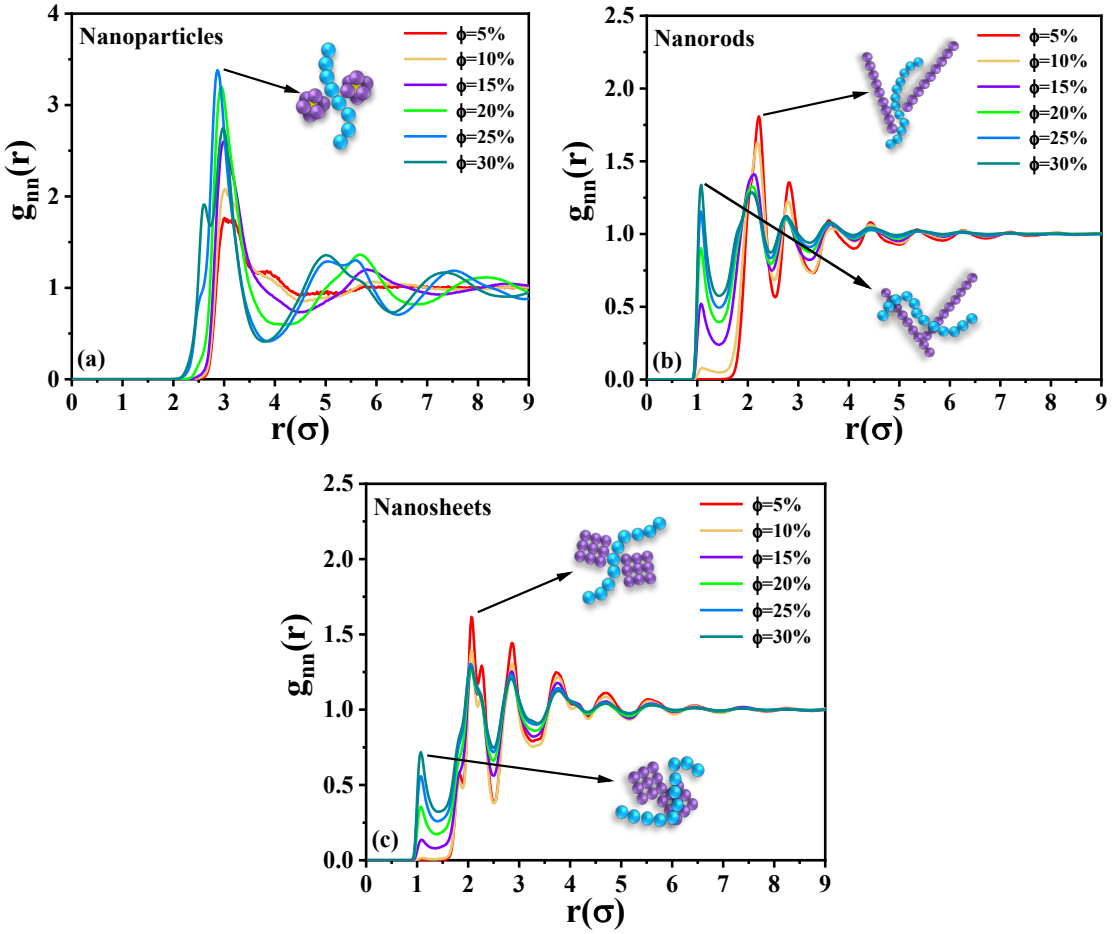
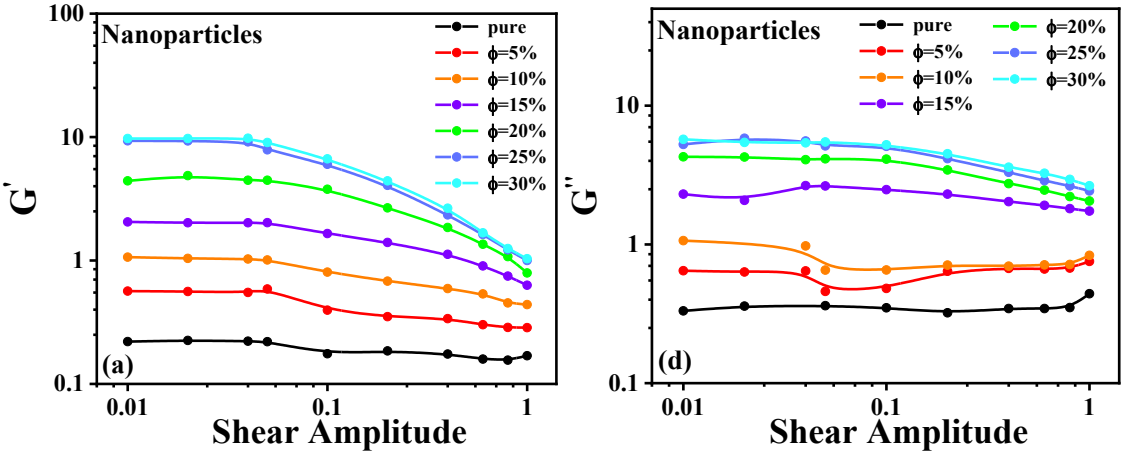


Fig. S1 RDF of PNCs respectively filled with (a) nanoparticles, (b) nanorods and (c) nanosheets at different filler volume fractions.



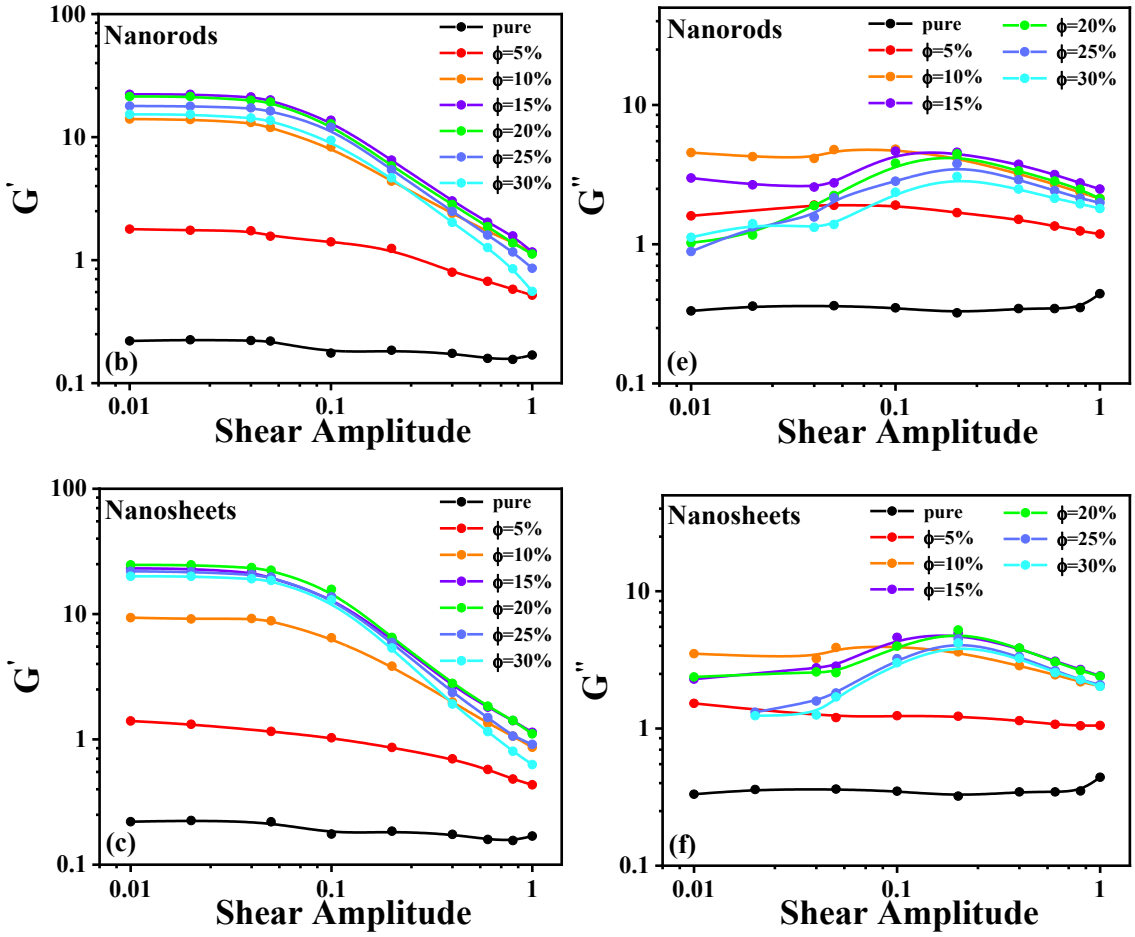
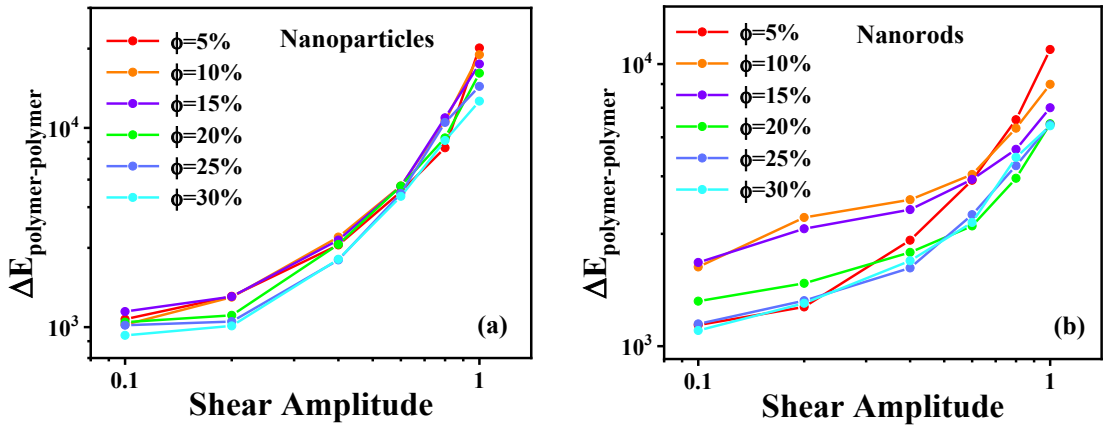


Fig. S2 Plots of energy storage modulus of PNCs respectively filled with (a) nanoparticles, (b) nanorods, (c) nanosheets and loss modulus of PNCs respectively filled with (d) nanoparticles, (e) nanorods, (f) nanosheets as a function of shear amplitude at different filler volume fractions. υ =0.01 τ^{-1}.



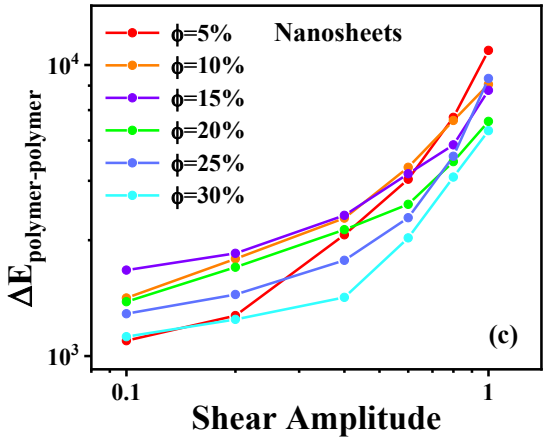


Fig. S3 Variation of polymer-polymer interaction energy difference with shear amplitude in PNCs respectively filled with (a) nanoparticles, (b) nanorods and (c) nanosheets at different filler volume fractions during oscillatory shear.

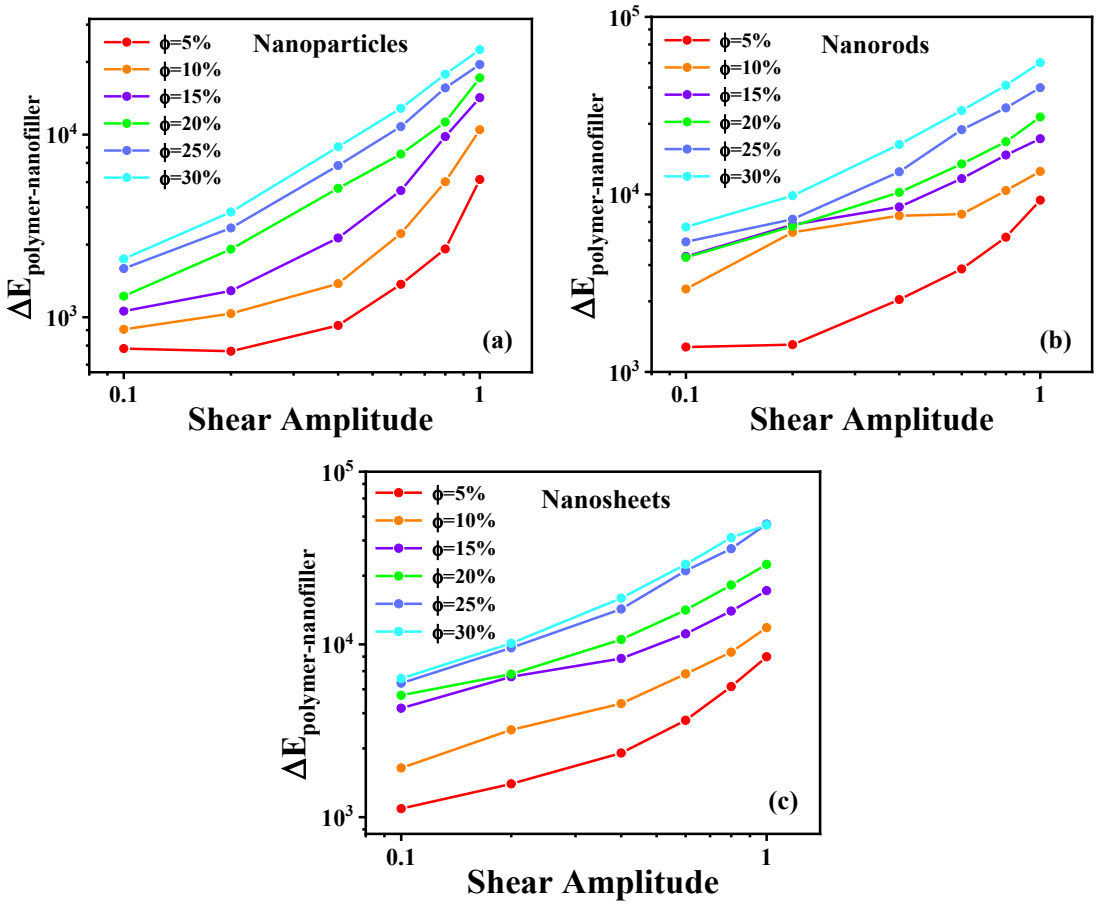


Fig. S4 Variation of polymer-filler interaction energy difference with shear amplitude in PNCs respectively filled with (a) nanoparticles, (b) nanorods and (c) nanosheets at different filler volume fractions during oscillatory shear.

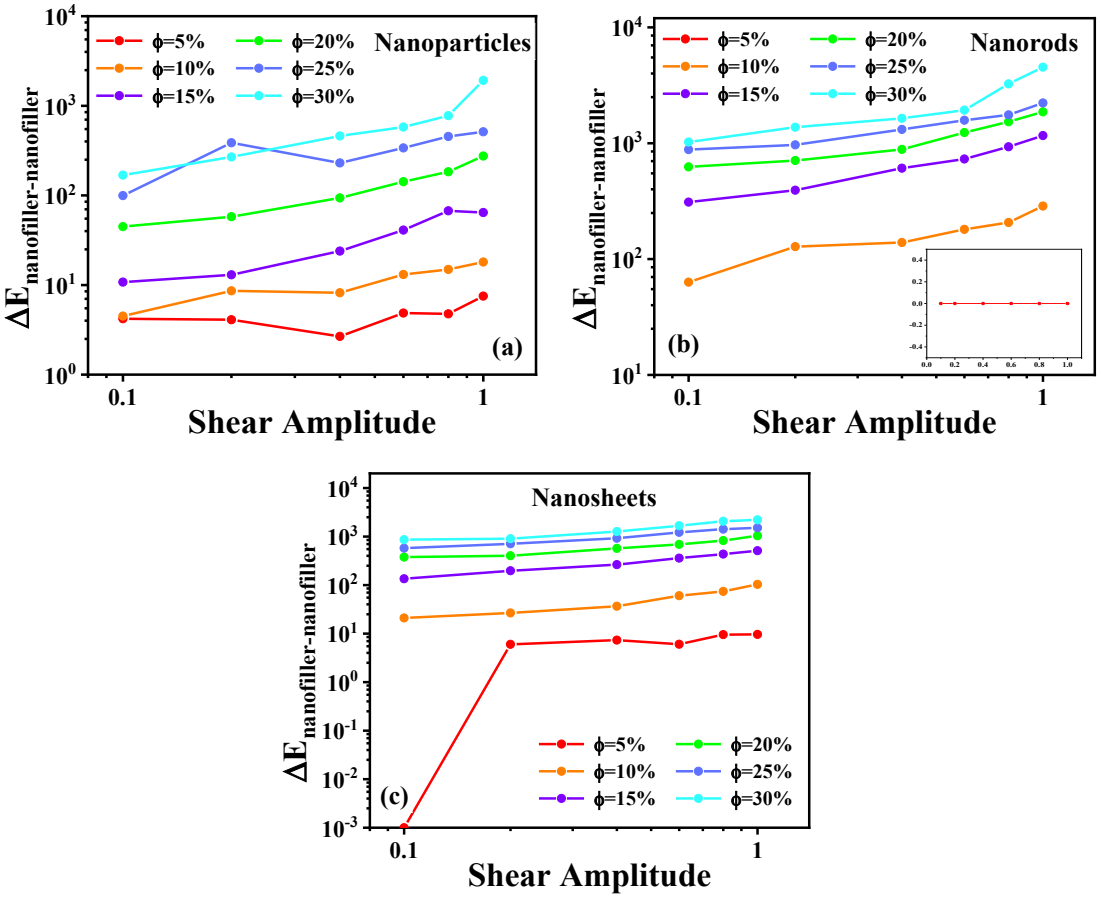
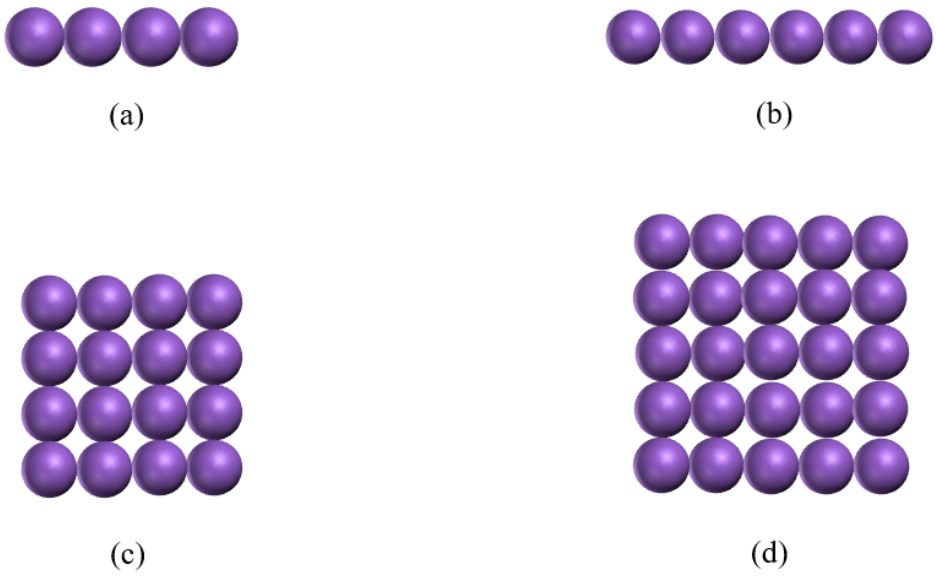


Fig. S5 Variation of filler-filler interaction energy difference with shear amplitude in PNCs respectively filled with (a) nanoparticles, (b) nanorods and (c) nanosheets at different filler volume fractions during oscillatory shear.



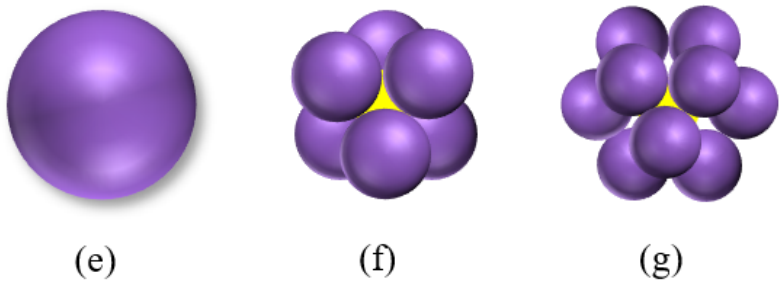


Fig. S6 Model snapshots of nanorods with filler size of (a) L=4 and (b) L=6, nanosheets with filler size of (c) 4×4 and (d) 5×5, (e) UNPs, (f) ONPs and (g) MNPs.

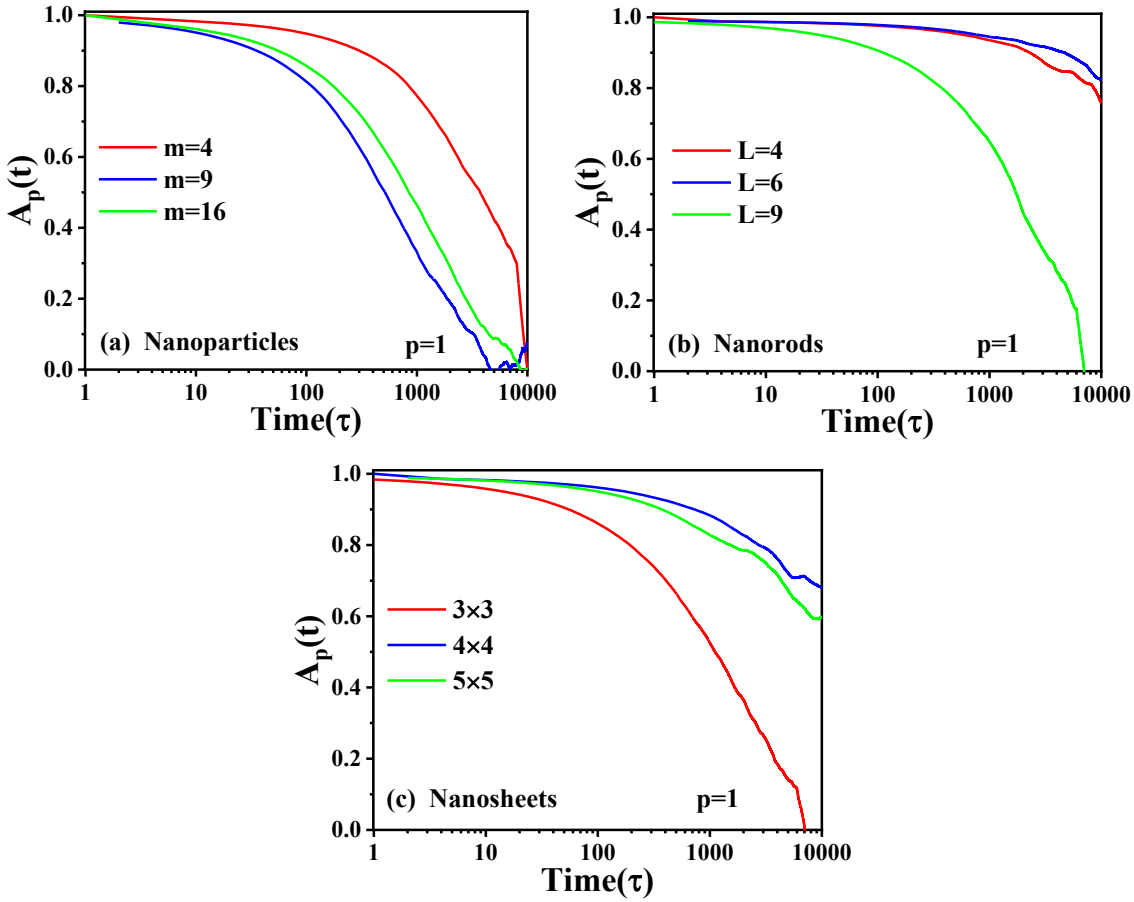


Fig. S7 Autocorrelation functions $A_p(t)$ for PNCs respectively filled with (a) nanoparticles, (b) nanorods and (c) nanosheets with different sizes at mode number p=1.

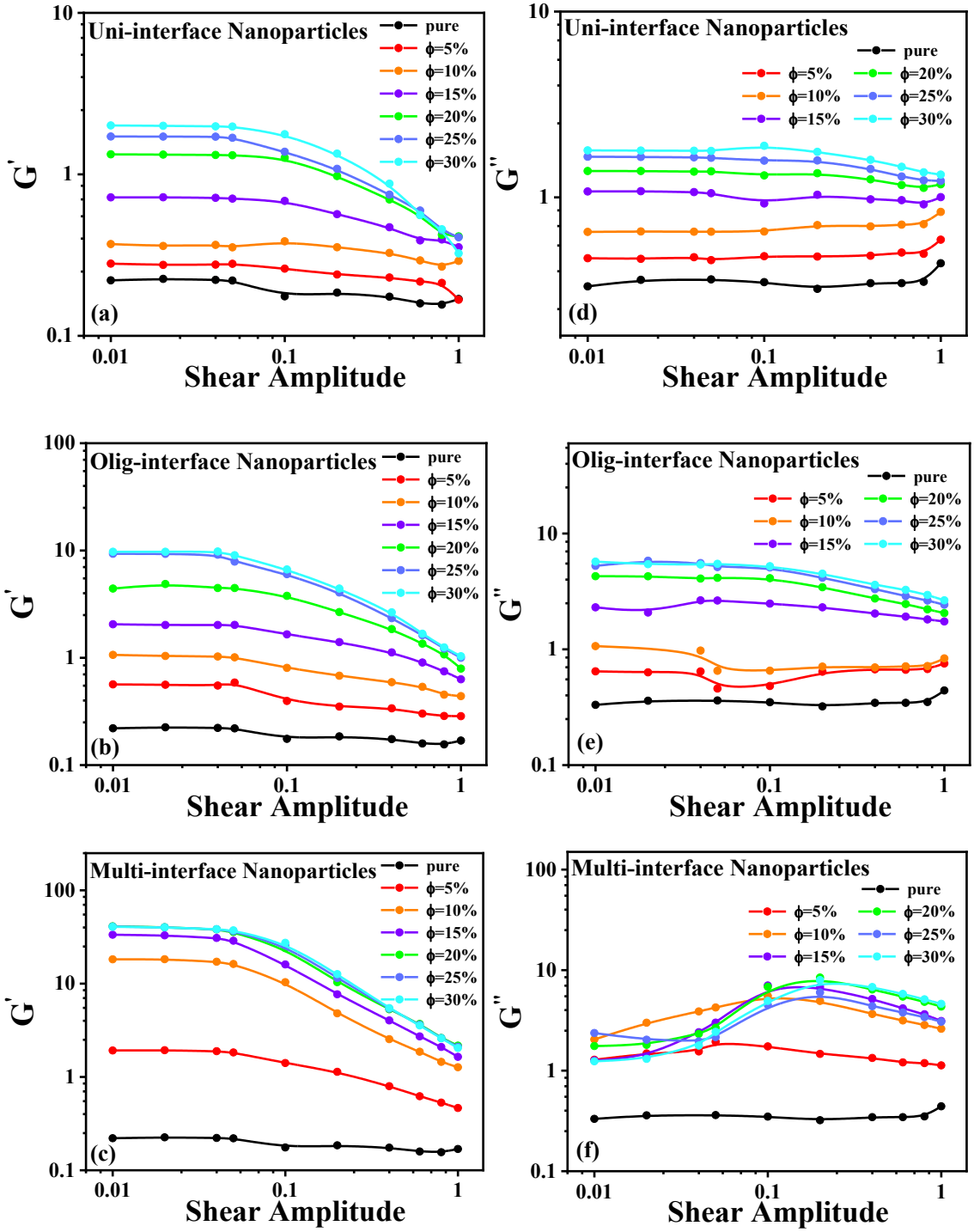


Fig. S8 Variation of energy storage modulus of PNCs respectively filled with (a) UNPs, (b) ONPs and (c) MNPs and loss modulus of PNCs respectively filled with (d) UNPs, (e) ONPs and (f) MNPs with shear amplitude at different filler volume fractions. $\upsilon = 0.01\,\tau^{-1}$.

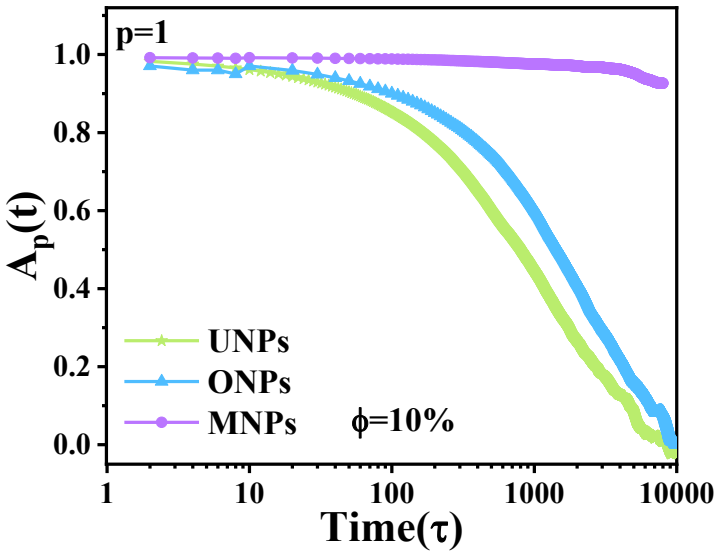


Fig. S9 Autocorrelation function $A_p(t)$ for PNCs respectively filled with different interfacial degrees nanoparticles at p=1.

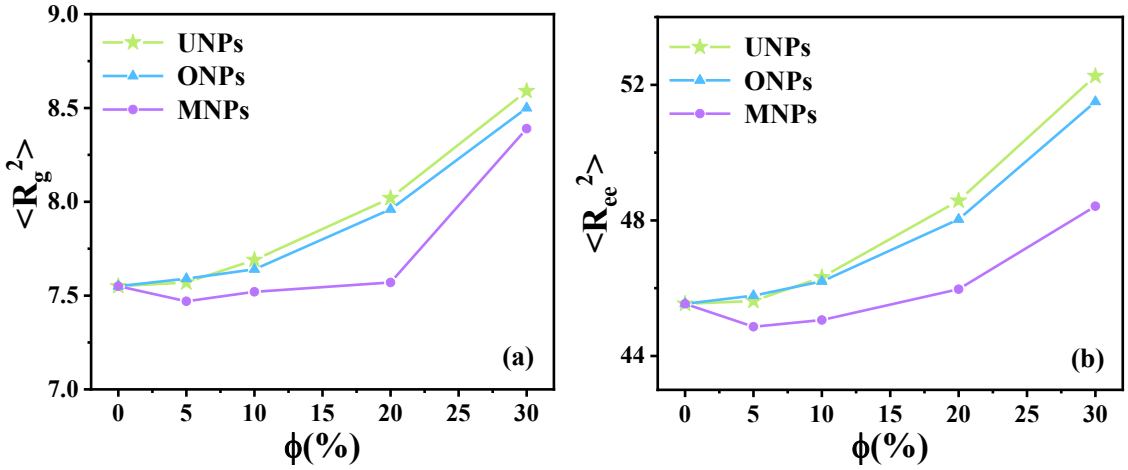


Fig. S10 Variation of (a) mean square radius of gyration and (b) mean square end distance with volume fraction for PNCs respectively filled with nanoparticles of different interfacial degrees.

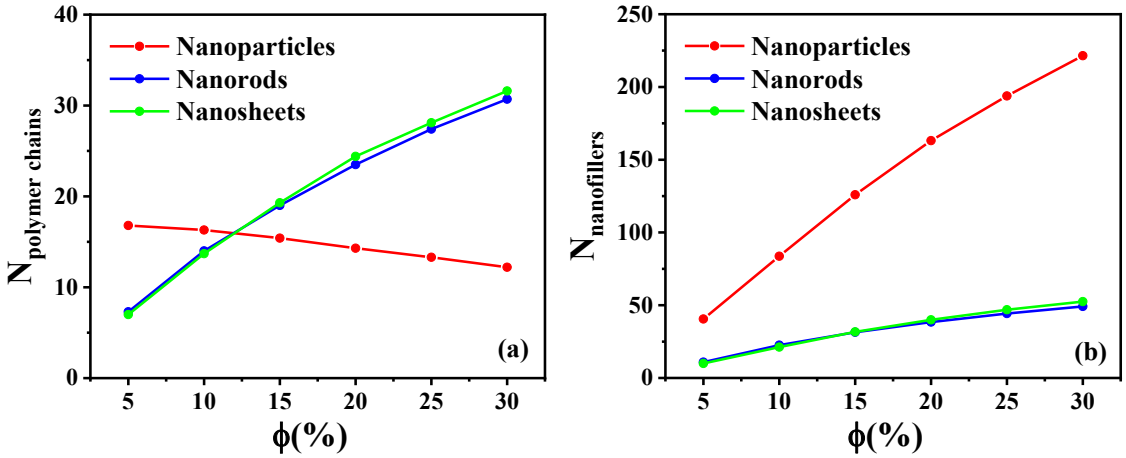


Fig. S11 (a) The average number of polymer chains associated with each nanofiller and (b) the average number of nanofillers associated with each polymer chain.

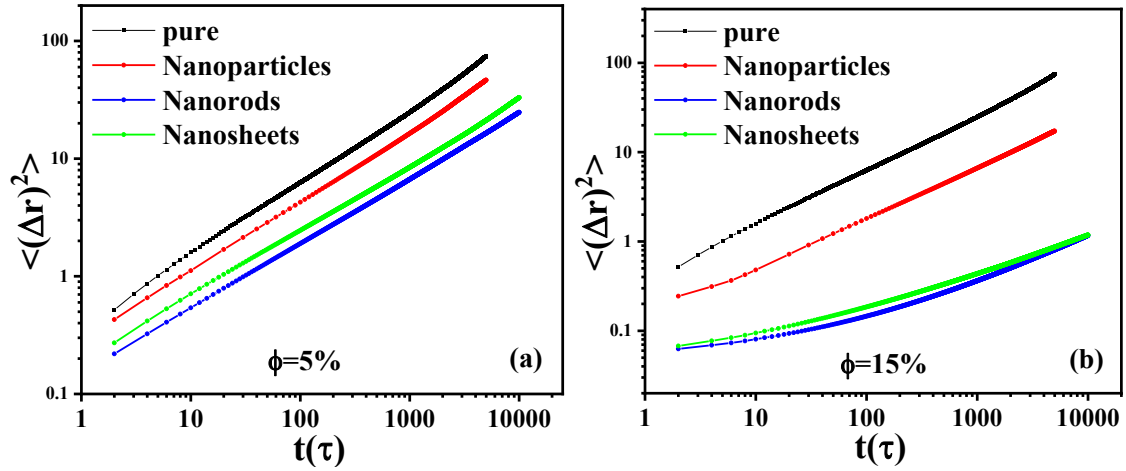


Fig. S12 MSD for pure polymer systems and different PNCs systems at (a) 5% and (b) 15% volume fraction.