

Supplementary Materials

Molecular Dynamics Simulation of Polymer Nanocomposites with Supramolecular Network Constructed via Functionalized Polymer End-Grafted Nanoparticles

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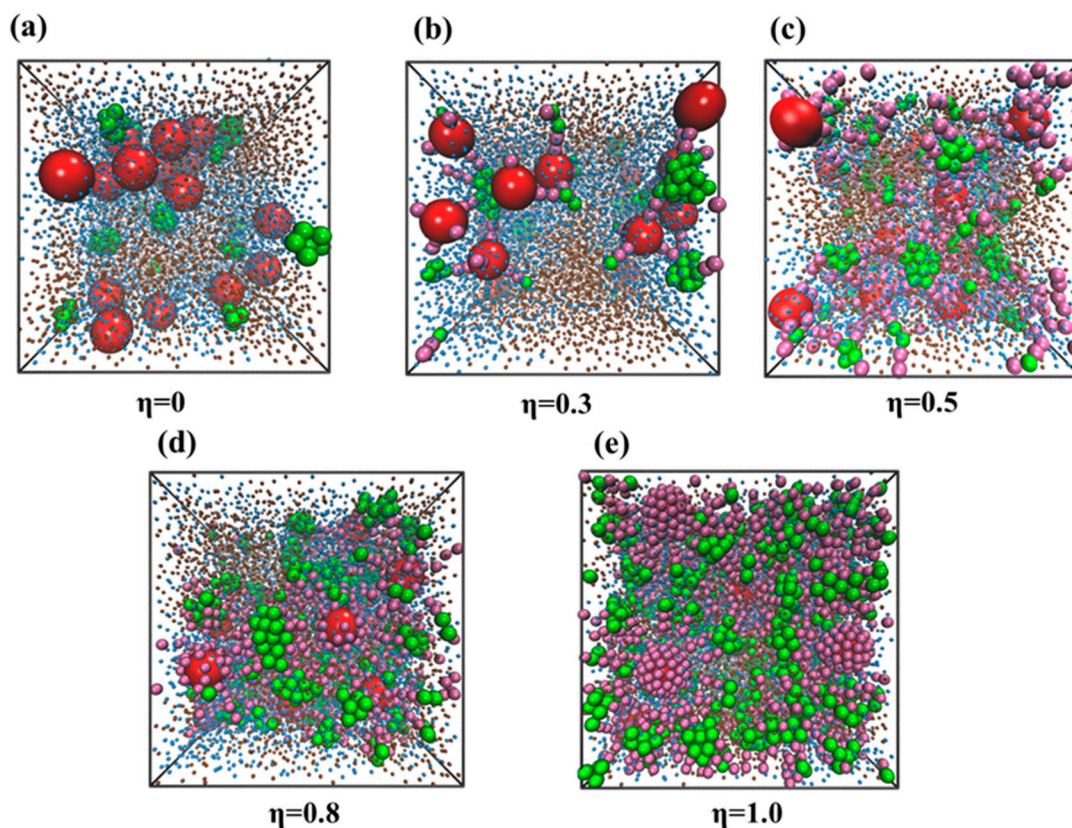


Figure S1. the snapshot of PNCs with different η , where: (a) $\eta = 0$; (b) $\eta = 0.3$; (c) $\eta = 0.5$; (d) $\eta = 0.8$;

(e) $\eta = 1.0$.

Table S1. the mean-square root radius of gyration of modified-NP (R_g)

| System | Mean-square root radius of gyration of modified-NP (σ) |
|--------------|--|
| $\eta = 0$ | 2.0 |
| $\eta = 0.3$ | 5.07 |
| $\eta = 0.5$ | 5.51 |
| $\eta = 0.8$ | 5.79 |
| $\eta = 1.0$ | 5.96 |

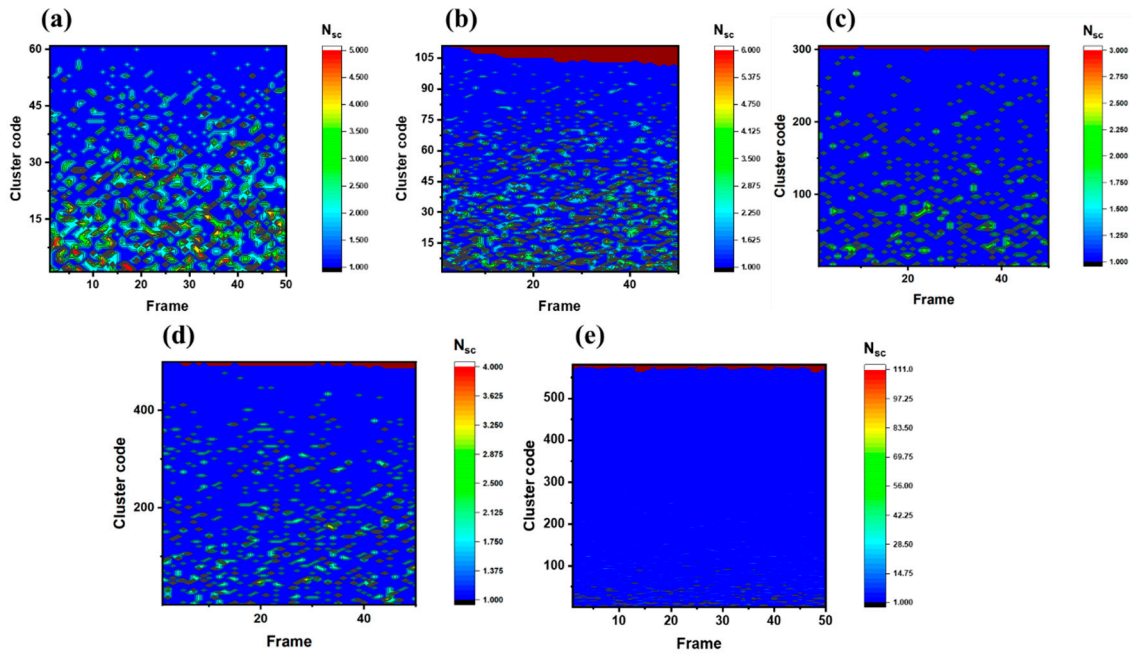


Figure S2. The size and distribution of clusters, which are formed by the modified group, with various sphericity (η) where (a) $\eta = 0$; (b) $\eta = 0.3$; (c) $\eta = 0.5$; (d) $\eta = 0.8$ and (e) $\eta = 1.0$.

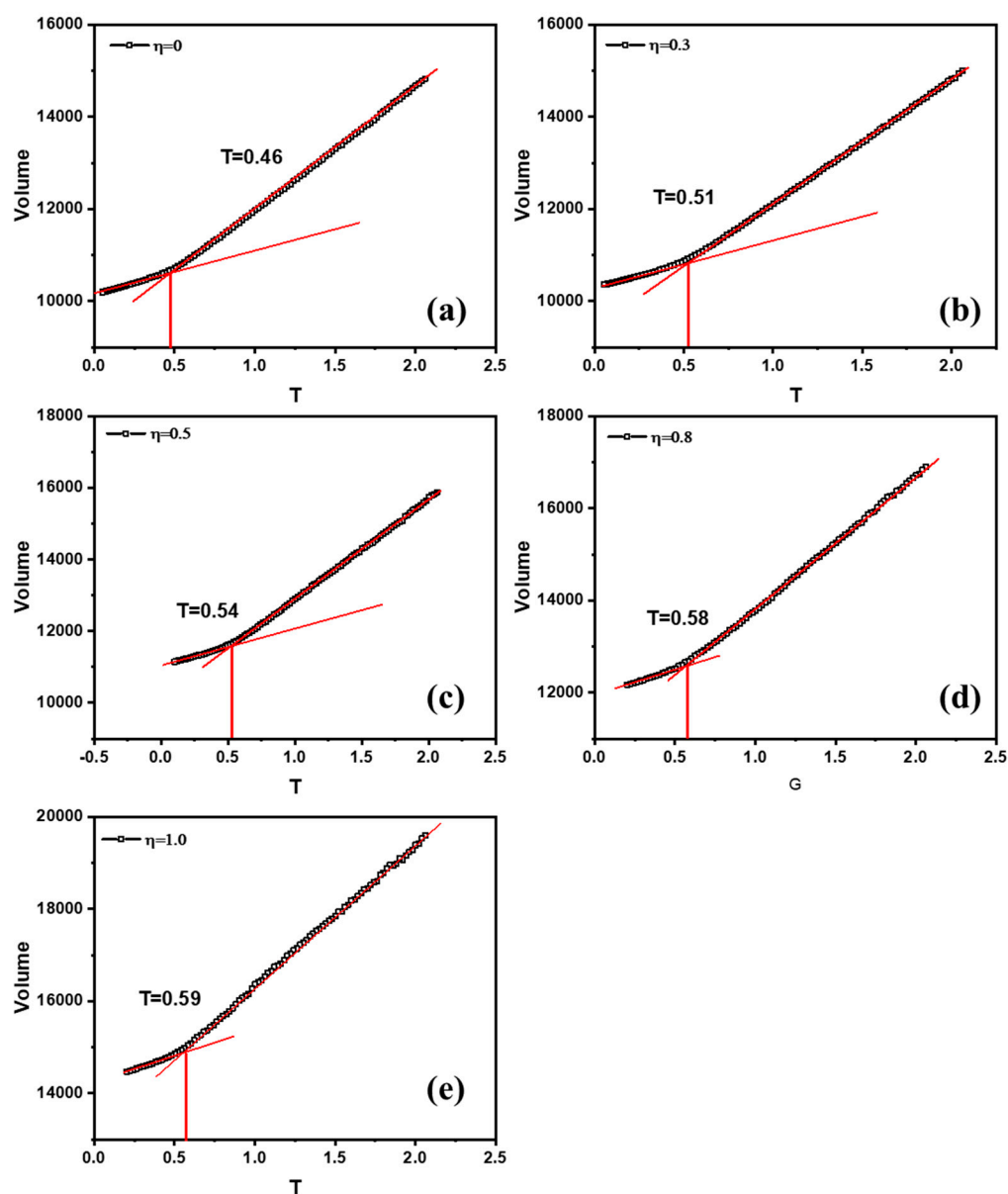


Figure S3. The glass transition temperature (T_g) obtained by the specific volume versus the temperature

for different η , where (a) $\eta = 0$; (b) $\eta = 0.3$; (c) $\eta = 0.5$; (d) $\eta = 0.8$ and (e) $\eta = 1.0$.