Supporting Information for:

Molecular dynamics simulation of self-assembly of one-component nanocrystals grafted with end-functionalized polymers

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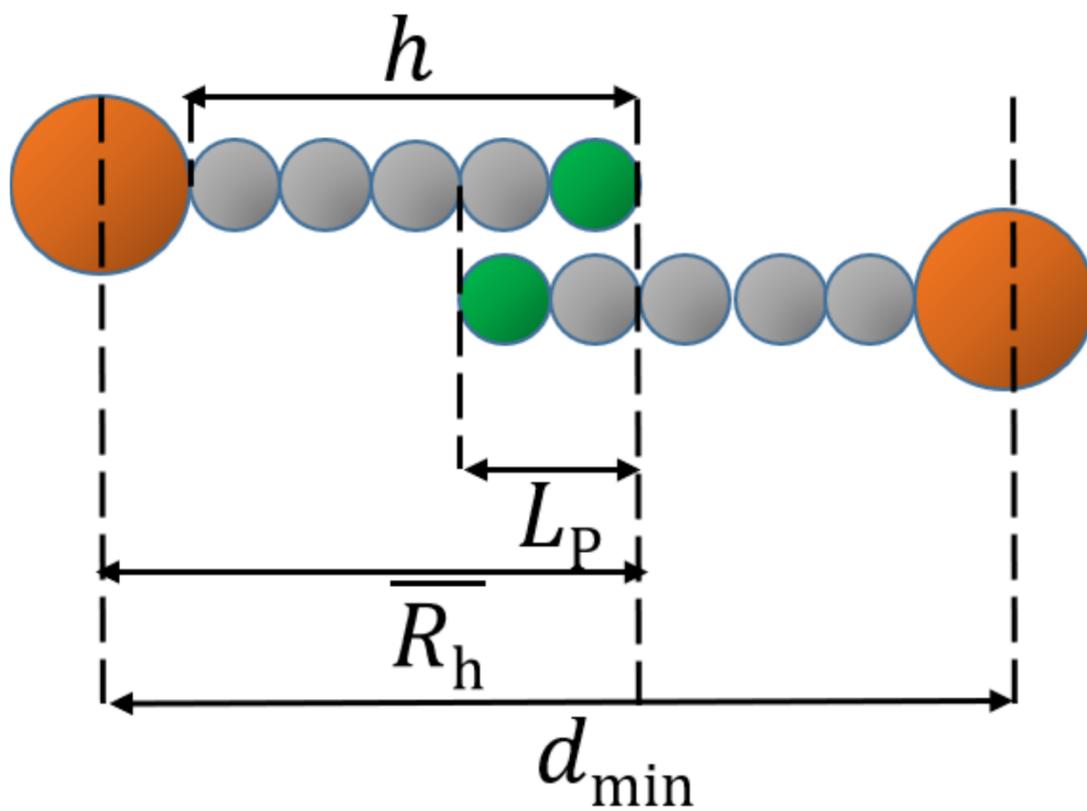
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Figure S1: Schematic illustration of the penetration degree P. The penetration degree P is defined as the ratio of the penetration length L_P to the polymer brush thickness h.
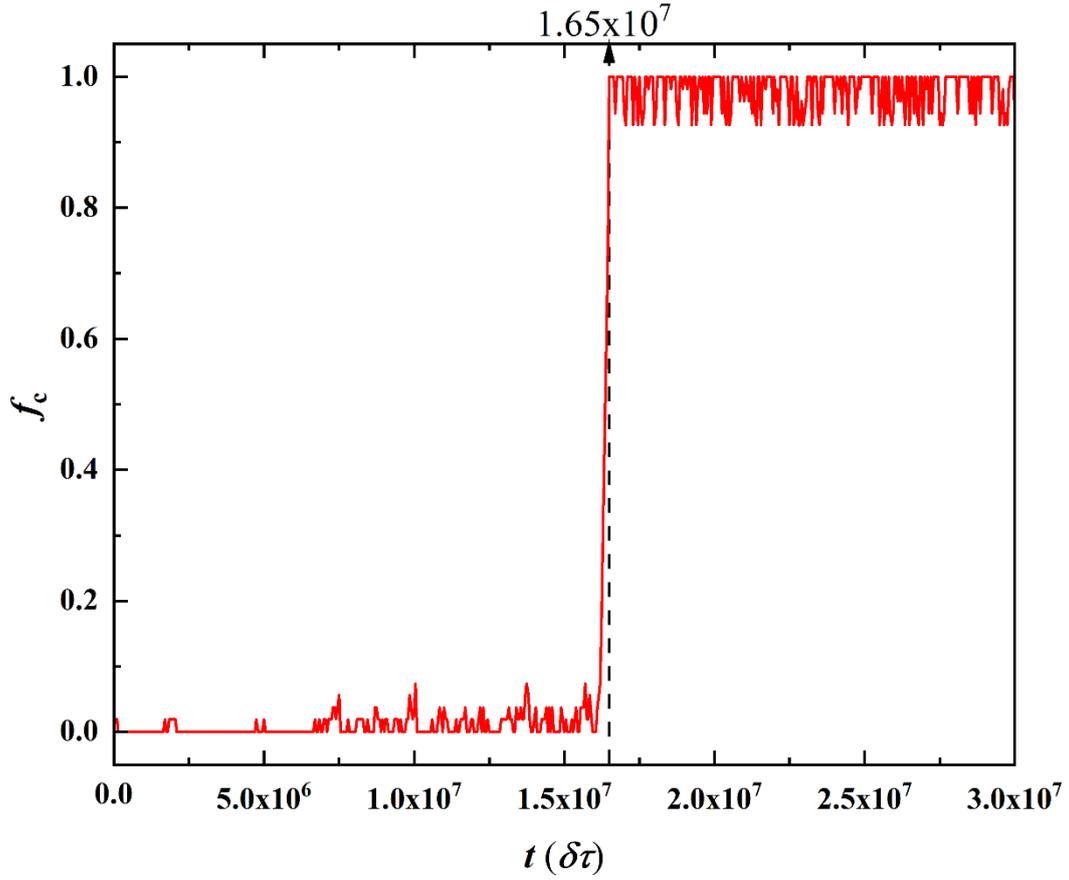
Figure S2: f_c as a function of simulation time t for a typical BCC superlattice ($\varepsilon_{aa} = 2$, $k_\theta = 20$, $N_L = 9$, $\sigma_g = 1.194$).
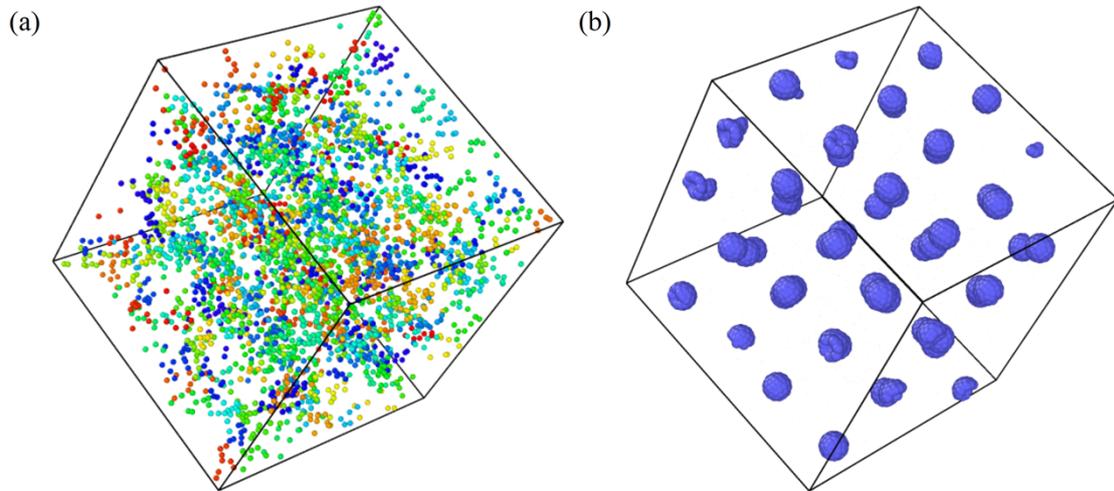

Figure S3: (a) Snapshot of cluster distribution and (b) Snapshot in a typical BCC superlattice system ($k = 359$) from the same perspective. Parameters for a typical BCC superlattice: $\varepsilon_{aa} = 2$, $k_\theta = 20$, $N_L = 9$, $\sigma_g = 1.194$.
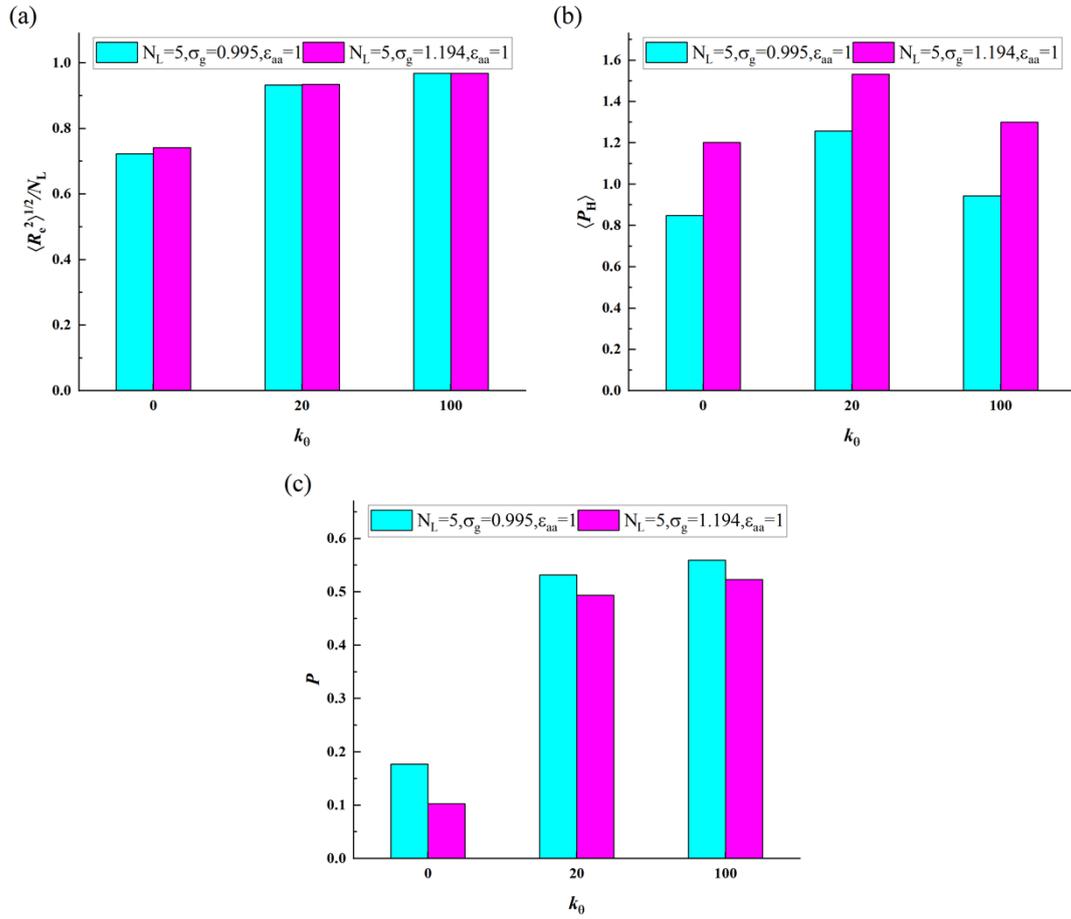
Figure S4: (a) $\langle R_e^2 \rangle^{1/2}/N_L$ as a function of chain rigidity k_θ, (b) $\langle P_H \rangle$ as a function of chain rigidity k_θ, (c) P as a function of chain rigidity k_θ.
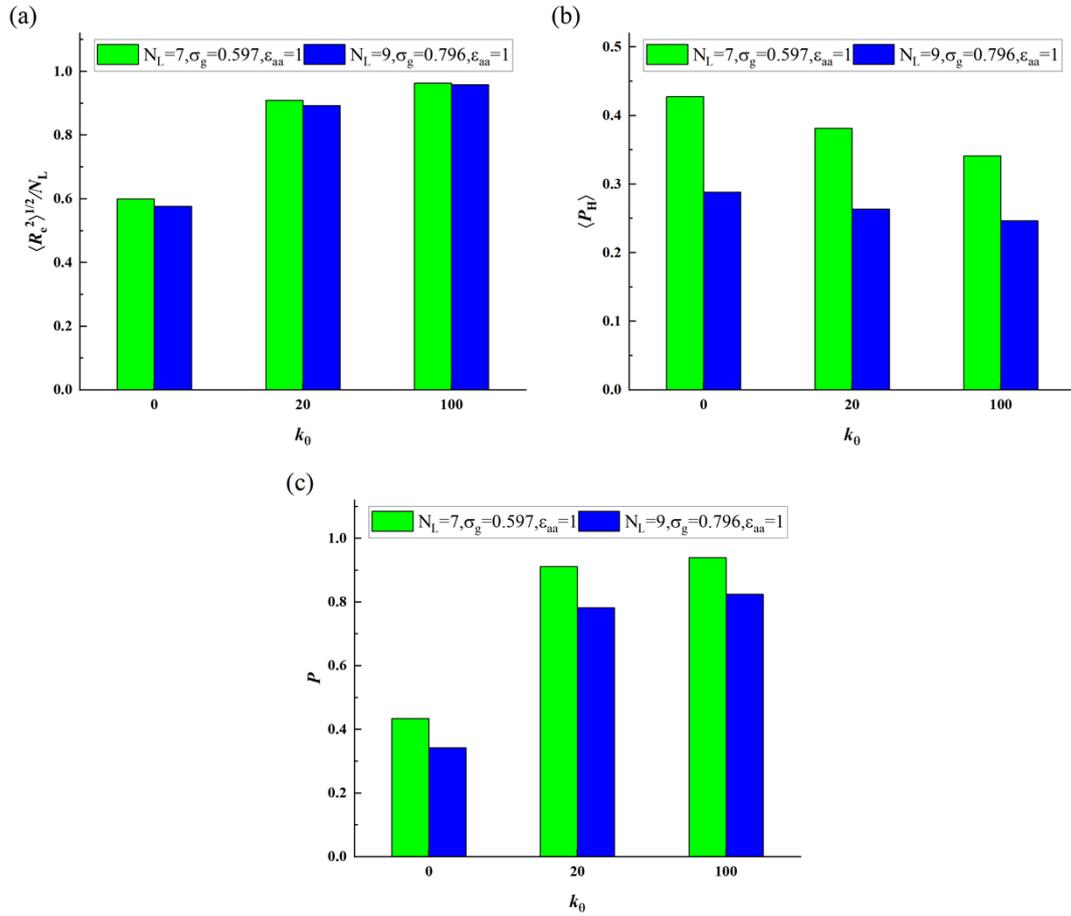
Figure S5: (a) $\langle R_e^2 \rangle^{1/2}/N_L$ as a function of chain rigidity k_θ, (b) $\langle P_H \rangle$ as a function of chain rigidity k_θ, (c) P as a function of chain rigidity k_θ.
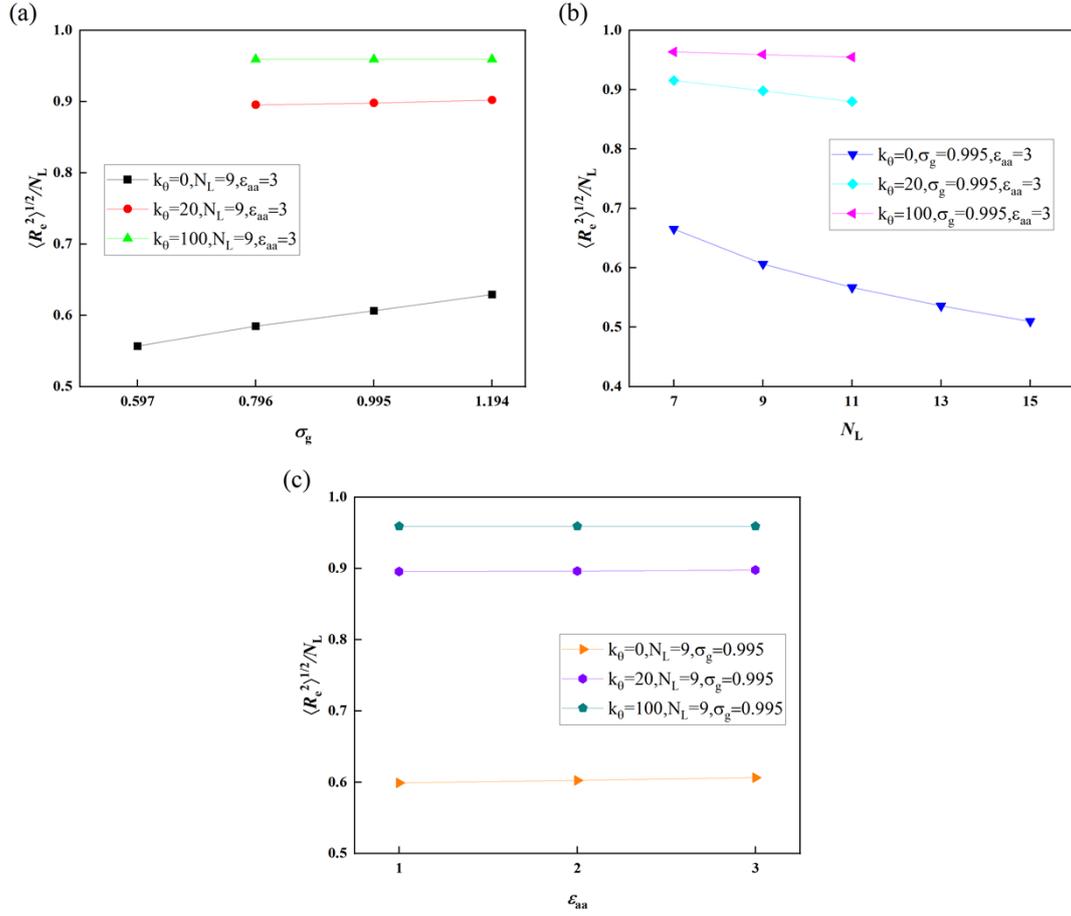
Figure S6: Under a series of chain rigidity k_θ ($k_\theta = 0, 20, 100$), (a) $\langle R_e^2 \rangle^{1/2}/N_L$ as a function of grafting density σ_g, (b) $\langle R_e^2 \rangle^{1/2}/N_L$ as a function of grafted chain length N_L, (c) $\langle R_e^2 \rangle^{1/2}/N_L$ as a function of potential well depth ε_{aa}.