# Impact of Free Energy of Polymers on Polymorphism of Polymer-Grafted Nanoparticles

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## Supporting Information

### A. Snapshots of PGNP

Figure S1 shows snapshots of PGNP before and after crystal phase transitions for $N = 20, 30, 50, 80, 100$.

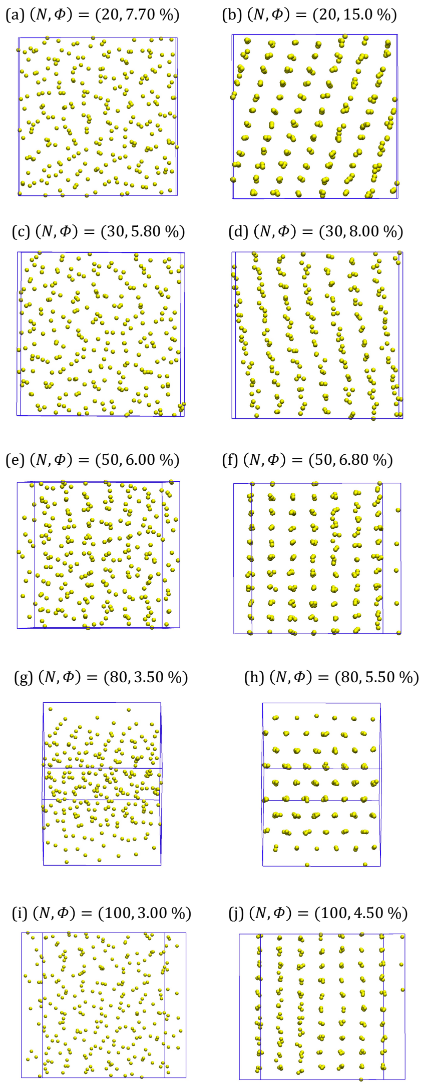


**Figure S1.** Snapshot of the system of PGNP before and after crystal phase transitions for $N = 20, 30, 50, 80, 100$. To help with the visualization of the structure of this phase, only cores of PGNP have been rendered, and core size and box size have been adjusted, respectively.

**B. Bond order parameter**

The distributions of the order parameters of each PGNP in the simulation box for $N = 30, 50, 80$ are shown in Figures S2, S3, S4, respectively.

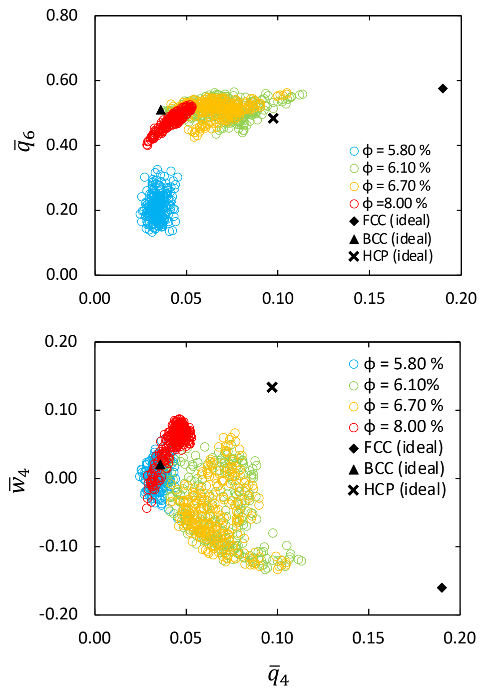


**Figure S2.** Plots of $\bar{q}_6$ **(top)** and $\bar{w}_4$ **(bottom)** versus $\bar{q}_4$ for $N = 30$, where all 256 PGNP point from each structure were chosen. The volume fraction of each point is denoted in the legend. For comparison, data points for perfect FCC, BCC and HCP crystals are also included.

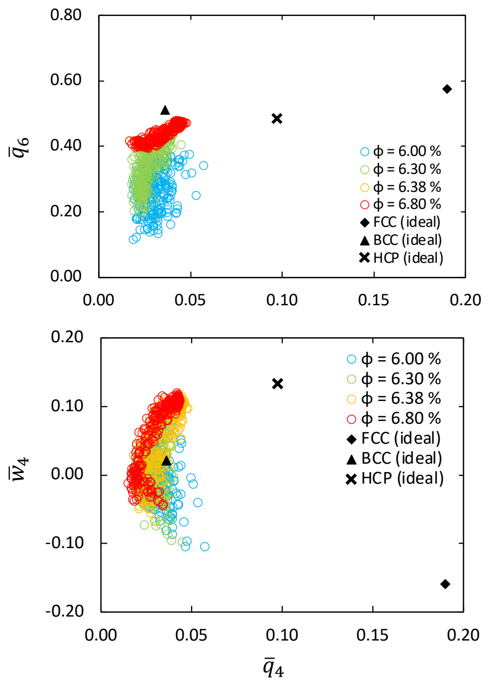


**Figure S3.** Plots of $\bar{q}_6$ **(top)** and $\bar{w}_4$ **(bottom)** versus $\bar{q}_4$ for $N = 50$, where all 256 PGNP point from each structure were chosen. The volume fraction of each point is denoted in the legend. For comparison, data points for perfect FCC, BCC and HCP crystals are also included.

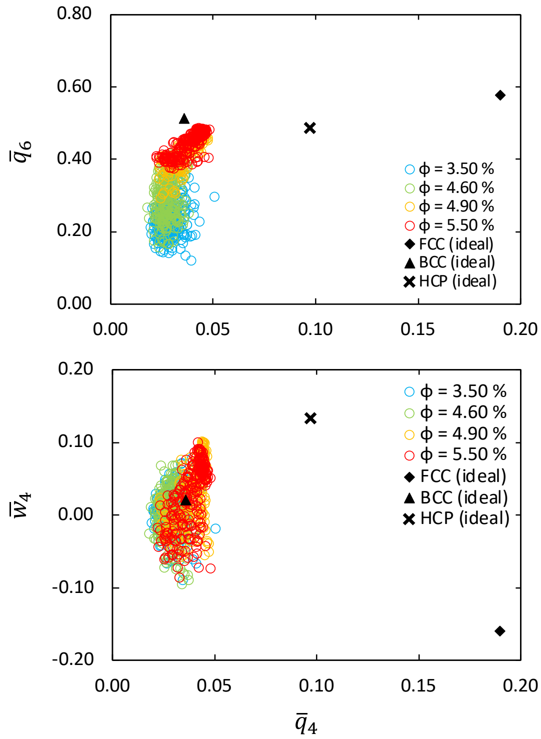


**Figure S4.** Plots of $\bar{q}_6$ **(top)** and $\bar{w}_4$ (**bottom**) versus $\bar{q}_4$ for $N = 80$, where all 256 PGNP point from each structure were chosen. The volume fraction of each point is denoted in the legend. For comparison, data points for perfect FCC, BCC and HCP crystals are also included.

### C. Relationship between $N$ and $R_g$ in dilute system

The relationship between $N$ and $R_g$ is expressed

$$R_g = bN^{\nu},$$

Where $b$ is Kuhn length and $\nu$ is the Flory exponent. Therefore, from the plots of $R_g$ versus $N$, $b$ and $\nu$ can be estimated. Figure S5 shows the plots of $N$ versus $< R_g^2 >$.

The regression line is

$$R_g = 0.408N^{0.674}$$

So, in this case, $b = 0.408$ and $\nu = 0.674$.

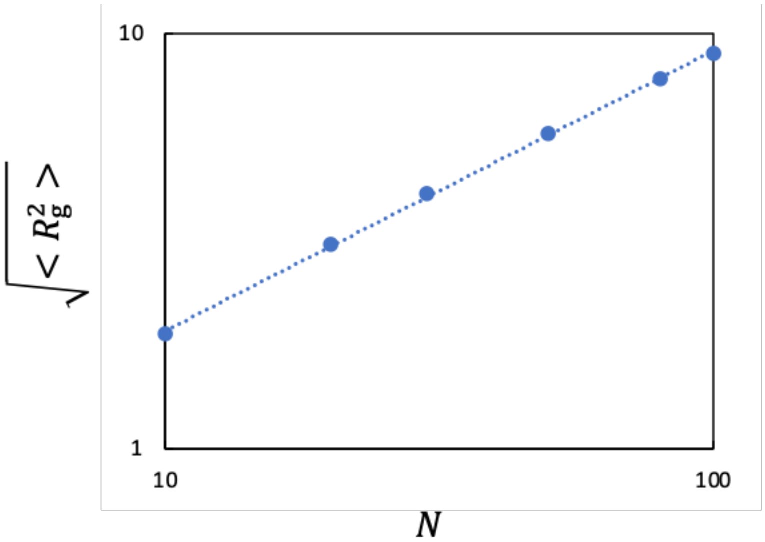


**Figure S5.** Plots of $\sqrt{< R_{\mathrm{g}}^2 >}$ versus $N$.