Supporting Information for Structure Factor of Blends of Solvent-Free Nanoparticle–Organic Hybrid Materials: Density-Functional Theory and Small Angle X-Ray Scattering

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S1 Parameter Calculations for Blends

Since our theory considers only bidisperse systems, we describe the blends using a bidisperse system that possesses the same statistical moments (mean and standard deviation of radius and grafting density, and third moment of grafting density) as the systems obtained by blending the theoretical description of the two pure systems (best-fit parameters: $\varepsilon_{\mathrm{core}}$, $\varepsilon_{\mathrm{core,eff}}$, $\varepsilon_{\mathrm{GD}}$, and a_{eff} for A and B). The theoretical input parameters for each blend include n_1, n_2, a_1, $a_{1,\mathrm{eff}}$, a_2, $a_{2,\mathrm{eff}}$, $\sigma_{\mathrm{s}1}$, and $\sigma_{\mathrm{s}2}$. For a given bulk number density (n_{b}) either n_1 or n_2 can be the independent variable that determines the mole fractions of the species 1 $(1-x_2)$ and 2 (x_2) in the model bidisperse system. Moreover, the overall deviation of S in the small-q regime from the monodisperse system is more sensitive to the variations in the oligomer grafting density. Therefore, for each blend we use the best-fit parameters for A and B to calculate a, a_{eff}, σ_{s}, $\varepsilon_{\mathrm{core}}$ (the standard deviation of core size), $\varepsilon_{\mathrm{GD}}$ (the standard deviation of grafting density), and $\mu_{3,\mathrm{GD}}$ (the third moment of grafting density) based on the know mixing ratio shown in Table 3, and use these statistical moments to directly obtain the input parameters for the model bidisperse system describing the blend. Specifically,

$$a = 0.5(1-x_{\mathrm{B}})\left(\sum_{i=1}^{2} a_i^{\mathrm{A}}\right) + 0.5x_{\mathrm{B}}\left(\sum_{i=1}^{2} a_i^{\mathrm{B}}\right), \tag{S1a}$$

$$\sigma_{\mathrm{s}} = 0.5(1-x_{\mathrm{B}})\left(\sum_{i=1}^{2} \sigma_{\mathrm{s}i}^{\mathrm{A}}\right) + 0.5x_{\mathrm{B}}\left(\sum_{i=1}^{2} \sigma_{\mathrm{s}i}^{\mathrm{B}}\right), \tag{S1b}$$

$$a_{\mathrm{eff}} = 0.5(1-x_{\mathrm{B}})\left(\sum_{i=1}^{2} a_{i,\mathrm{eff}}^{\mathrm{A}}\right) + 0.5x_{\mathrm{B}}\left(\sum_{i=1}^{2} a_{i,\mathrm{eff}}^{\mathrm{B}}\right), \tag{S1c}$$

$$\varepsilon_{\mathrm{core}} = \frac{1}{a}\sqrt{0.5(1-x_{\mathrm{B}})\left[\sum_{i=1}^{2}\left(a_i^{\mathrm{A}}-a\right)^2\right] + 0.5x_{\mathrm{B}}\left[\sum_{i=1}^{2}\left(a_i^{\mathrm{B}}-a\right)^2\right]}, \tag{S1d}$$

$$\varepsilon_{\mathrm{core,eff}} = \frac{1}{a_{\mathrm{eff}}}\sqrt{0.5(1-x_{\mathrm{B}})\left[\sum_{i=1}^{2}\left(a_{i,\mathrm{eff}}^{\mathrm{A}}-a_{\mathrm{eff}}\right)^2\right] + 0.5x_{\mathrm{B}}\left[\sum_{i=1}^{2}\left(a_{i,\mathrm{eff}}^{\mathrm{B}}-a_{\mathrm{eff}}\right)^2\right]}, \tag{S1e}$$

$$\varepsilon_{\mathrm{GD}} = \frac{1}{\sigma_{\mathrm{s}}}\sqrt{0.5(1-x_{\mathrm{B}})\left[\sum_{i=1}^{2}\left(\sigma_{\mathrm{s}i}^{\mathrm{A}}-\sigma_{\mathrm{s}}\right)^2\right] + 0.5x_{\mathrm{B}}\left[\sum_{i=1}^{2}\left(\sigma_{\mathrm{s}i}^{\mathrm{B}}-\sigma_{\mathrm{s}}\right)^2\right]}, \tag{S1f}$$

$$\mu_{3,\mathrm{GD}} = 0.5(1-x_{\mathrm{B}})\left[\sum_{i=1}^{2}\left(\sigma_{\mathrm{s}i}^{\mathrm{A}}-\sigma_{\mathrm{s}}\right)^3\right] + 0.5x_{\mathrm{B}}\left[\sum_{i=1}^{2}\left(\sigma_{\mathrm{s}i}^{\mathrm{B}}-\sigma_{\mathrm{s}}\right)^3\right], \tag{S1g}$$

where superscripts A and B represent parameters for samples A and B. The parameters for the model bidisperse system (x_2, a_1, $a_{1,\mathrm{eff}}$, a_2, $a_{2,\mathrm{eff}}$, σ_{s1}, and σ_{s2}) are then obtained by simultaneously solving

$$a = (1-x_2)a_1 + x_2 a_2, \tag{S2a}$$

$$a_{\mathrm{eff}} = (1-x_2)a_{1,\mathrm{eff}} + x_2 a_{2,\mathrm{eff}}, \tag{S2b}$$

$$\sigma_{\mathrm{s}} = (1-x_2)\sigma_{\mathrm{s}1} + x_2 \sigma_{\mathrm{s}2}, \tag{S2c}$$

$$\varepsilon_{\mathrm{core}} = \frac{1}{a}\sqrt{(1-x_2)\,(a_1-a)^2 + x_2\,(a_2-a)^2}, \tag{S2d}$$

$$\varepsilon_{\mathrm{core,eff}} = \frac{1}{a_{\mathrm{eff}}}\sqrt{(1-x_2)\left(a_{1,\mathrm{eff}}-a_{\mathrm{eff}}\right)^2 + x_2\left(a_{2,\mathrm{eff}}-a_{\mathrm{eff}}\right)^2}, \tag{S2e}$$

$$\varepsilon_{\mathrm{GD}} = \frac{1}{\sigma_{\mathrm{s}}}\sqrt{(1-x_2)\,(\sigma_{\mathrm{s}1}-\sigma)^2 + x_2\,(\sigma_{\mathrm{s}2}-\sigma_{\mathrm{s}})^2}, \tag{S2f}$$

$$\mu_{3,\mathrm{GD}} = (1-x_2)\,(\sigma_{\mathrm{s}1}-\sigma_{\mathrm{s}})^3 + x_2\,(\sigma_{\mathrm{s}2}-\sigma_{\mathrm{s}})^3. \tag{S2g}$$