Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information:

Polymer-nanoparticle interfacial behavior revisited: A molecular dynamics study

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This supporting information provides filler-bead radial distribution function for different polymer-filler interactions, the mean square radius of gyration R_g^2, the change of the position of a chosen representative polymer chain and the radial distribution function (RDF) between nanoparticles

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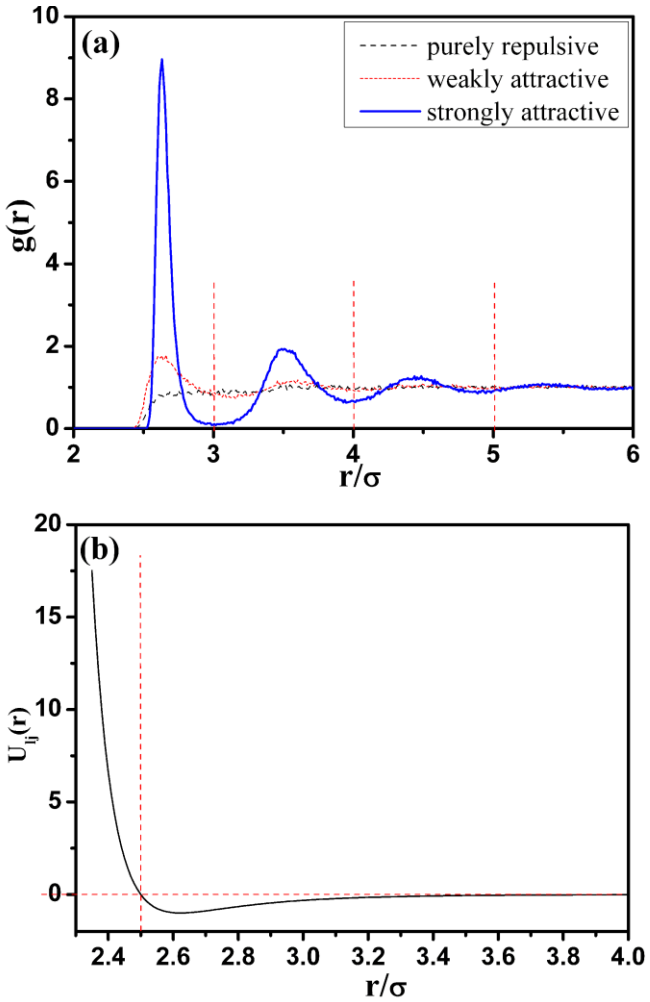

Figure S1 (a)The filler-bead radial distribution function for different polymer-filler interactions. (b)Sketch of the van der Waals forcefield for the polymer-filler interaction. Note that the purely repulsive, weakly and strongly attractive polymer-filler interactions respectively stands for (i) $\varepsilon_{np}=1.0$ **and** $r_{cutoff}=1.12$ **; (ii)** $\varepsilon_{np}=1.0$ **and** $r_{cutoff}=2.5$ **; (iii)** $\varepsilon_{np}=10.0$ **and** $r_{cutoff}=2.5$**.**

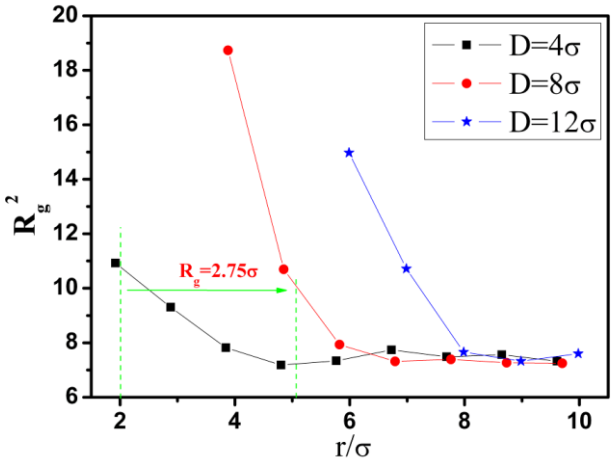

Figure S2 The mean square radius of gyration R_g^2 as a function the distance between the chain center of mass and the filler center for three different filler sizes. Notedly the length scale of the perturbed region from the filler surface is approximately the polymer dimension R_g.

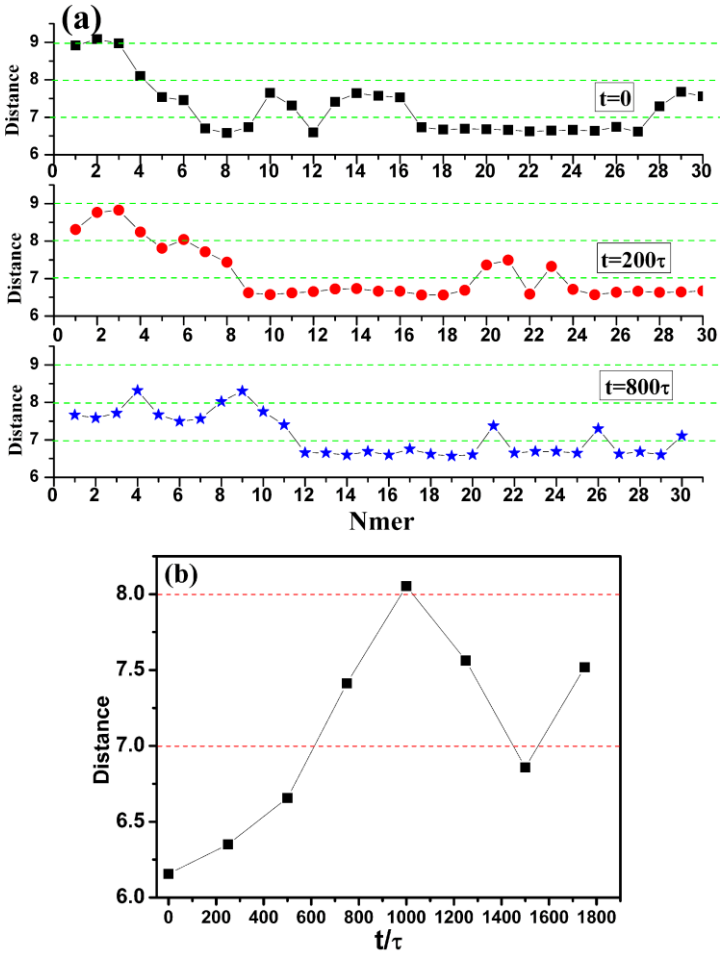

Figure S3 (a)The change of the position of a chosen representative polymer chain, initially adsorbed in the interfacial region as a function of time. (b) The corresponding change of the distance between the mass center of this polymer chain and the filler center. Note that the diameter of the nanoparticle is D=12σ .

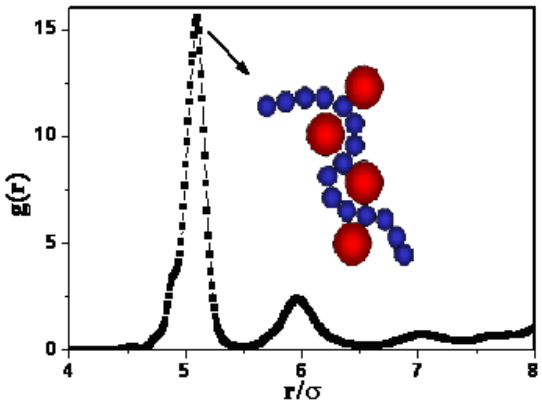

Figure S4 The radial distribution function (RDF) between nanoparticles, with its volume fraction equal to $\varphi = 18.55\%$ and size $D = 4\sigma$, and the polymer-filler interaction strength is $\varepsilon_{pn} = 10.0$.