Supplementary Material for Soft Matter

Entanglements in polymer nanocomposites containing spherical nanoparticles

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TABLE S1: Nanoparticle volume fraction ϕ $(\%)$, length of the simulation cell (L) measured in units of the monomer diameter σ_m, nanoparticles of radius R and $type$: repulsive (Re), attractive (A), polymer matrix:$N = 200$, N_e(S-coil, S-kink, modified S-coil, M-coil), number of "kinks" $< Z >$ in the frozen limit, number of "kinks" $< Z >$(phantom) in the phantom limit, L_{pp}: contour length of the primitive path in the frozen limit, L_{pp}(phantom): contour length of the primitive path in the phantom limit. Tube diameter α_{pp} of polymers with $N = 200$ in the nanocomposites. The error bar is the standard deviation

ϕ (%)	$L(\sigma_m)$	$type$	(S-coil)	(S-kink)	(m.S-coil)	(M-coil)	$< Z >$	$< Z >$(phantom)	L_{pp}	L_{pp}(phantom)	α_{pp}
26.6	33.416	Re ($R = 4$)	60.8±2.6	32.9±1.6	80.5±4.6		5.1±0.3	5±0.2	37.7±0.7	-	-
26.95	33.343	A ($R = 4$)	62.5±3.9	32.6±1.5	83.9±7.4	57.4	5.2±0.3	4.9±0.1	37.6±0.7	36.9±0.5	11.95
19.5	32.531	Re ($R = 4$)	60.9±2.5	32.6±1.4	80.2±4.6		5.5±0.3	5.0±0.1	36.7±1.0	-	-
19.6	32.458	A ($R = 4$)	60±2.4	32±1.3	78.3±4.1	66.4	5.3±0.3	5.1±0.2	37.6±0.6	37.4±0.6	10.987
10.3	31.534	Re ($R = 4$)	63.2±1.7	33.7±0.9	83.6±3.2		4.9±0.2	4.9±0.2	36±0.6	-	-
10.7	31.386	A ($R = 4$)	55.2±2.2	32.2±1.0	69.8±3.8		5.2±0.2	5.1±0.2	37.2±0.5	36.9±0.6	10.205
25.4	34.068	Re ($R = 2$)	60.9±2.7	33.5±0.9	80±4.8		4.9±0.2	4.9±0.1	36.3 ±4.8	-	-
25.8	33.909	A ($R = 2$)	66.1±2.4	31.8±1	90.7±4.7	64	5.3±0.2	4.5±0.2	39.5±0.6	37.7±0.5	12.825
18.7	32.963	Re ($R = 2$)	61.9±2.9	33.8±1.1	81.6±5.1		4.9±0.2	4.8±0.2	36±0.6	-	-
19	32.780	A ($R = 2$)	64.4±2.7	30.3±0.9	88.1±5.2	63.4	5.6±0.2	5.1±0.2	39.7±0.8	38.6±0.7	11.255
10.5	31.766	Re ($R = 2$)	61±3	33.5±1.1	80.2±5.4		5±0.2	4.9±0.2	36.1±0.8	-	-
10.6	31.636	A ($R = 2$)	57.6±2.2	32.3±1.0	74.5±3.8		5.2±0.2	5±0.2	37.5±0.6	37.1±0.5	10.393

TABLE S2: Nanoparticle volume fraction ϕ (%), nanoparticles of radius $R = 1$ and $type$: repulsive (Re), attractive (A), polymer matrix:$N = 200$, Entanglement length, N_e, extracted by the M-coil estimator, L_{pp}(phantom): contour length of the primitive path in the phantom limit, L_{pp}: contour length of the primitive path in the frozen limit, Tube diameter α_{pp} of polymers with $N = 200$ in the nanocomposites.The error bar is the standard deviation.

ϕ (%)	L	$type$	N_e(M-coil)	L_{pp} (phantom)	L_{pp}	α_{pp}
36	38.53	A	14	-	85.7	-
22.9	35.267	Re	-	33.1±0.5	63.6±2.6	11.058
24.2	34.653	A	21.2	37.5±0.5	67.6±2.3	14.235
17.3	33.831	Re	-	36±0.5	46.1±4.7	10.436
18.2	33.282	A	33.6	38.1±0.7	56.5±4.4	13.1
13.8	33.117	Re	-	35.1±1	41.2±2.1	10.801
14.5	32.568	A	41.9	37.2±0.6	46.7±2.9	11.369
10	32.280	Re	-	36.5±0.7	40.5±1.0	10.375
10.3	31.863	A	49.2	37.5±0.6	42.1±0.9	10.608
5.4	31.398	Re	-	36.6±0.8	38.1±0.8	10.011
5.5	31.157	A	55.64	38.3±0.6	39.9±0.6	9.879

TABLE S3: Contour length of the primitive path in the frozen limit, L_{pp}, in nanocomposites containing attractive nanoparticles of radius $R = 1$ and polymer matrices $N < 200$. Nanoparticle volume fractions ϕ (%) and polymer matrices N.

ϕ (%)	L_{pp} ($N = 10$)	L_{pp} ($N = 20$)	L_{pp} ($N = 50$)	L_{pp} ($N = 100$)
36	4.6	8.7	21.2	44
24.2	4.1	7.3	16.8	33.6
18.2	3.8	5.9	13.7	29.4
14.5	3.9	6.4	13.2	25
10.3	3.9	6.2	12.5	22.8
5.5	3.8	6	11.7	21.6

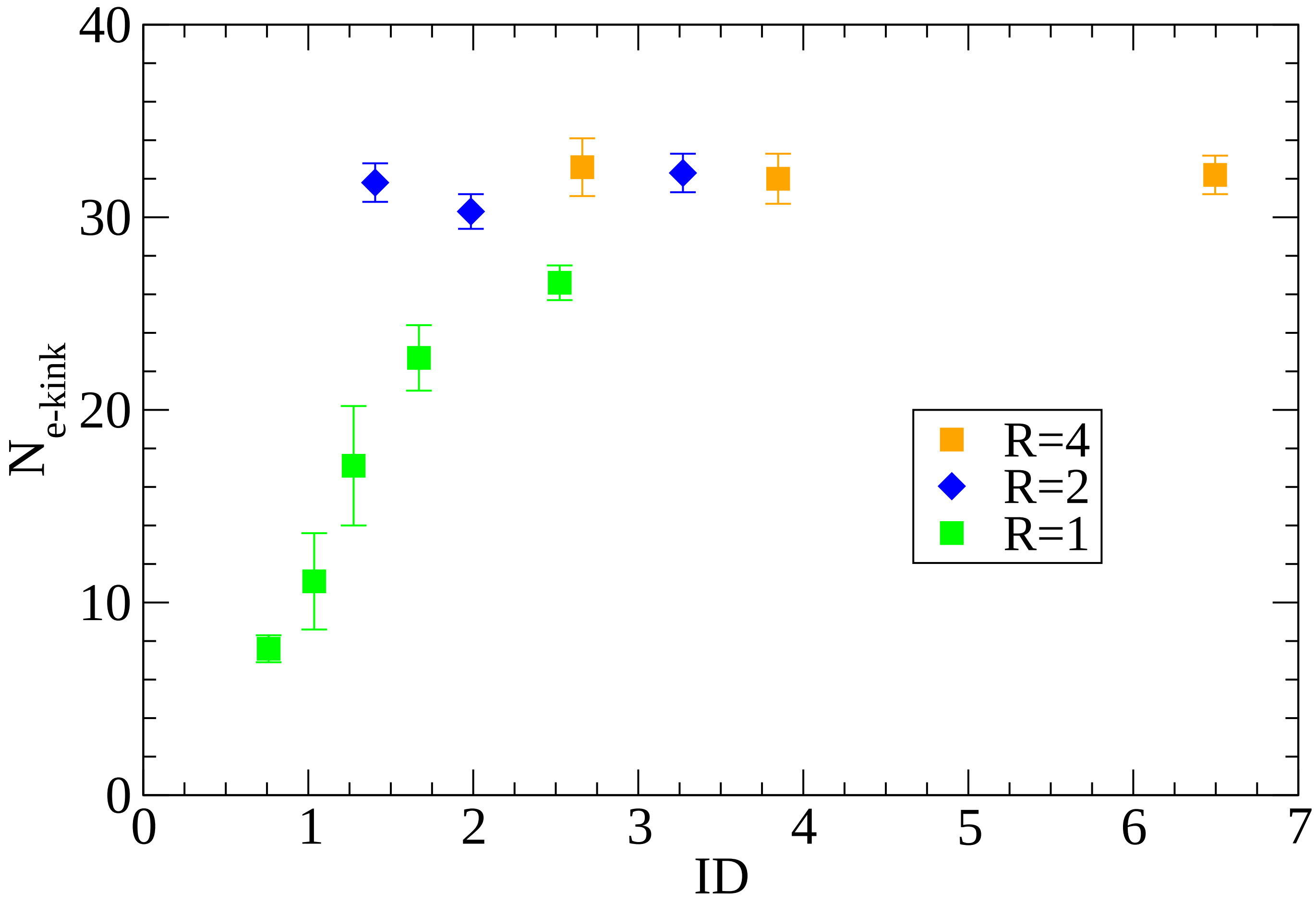

FIG. S1: Entanglement length N_e predicted by Eq.2 for the nanocomposites as a function of the interparticle distance ID for different nanoparticle sizes. Predictions of the entanglement length by Eq. 1 follow the same trends.