
Supporting Information:

Nanocomposite of Fullerenes and Natural Rubbers: MARTINI Force Field Molecular Dynamics Simulations

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Table S1: Details of the CG force field for *cis*-PI.

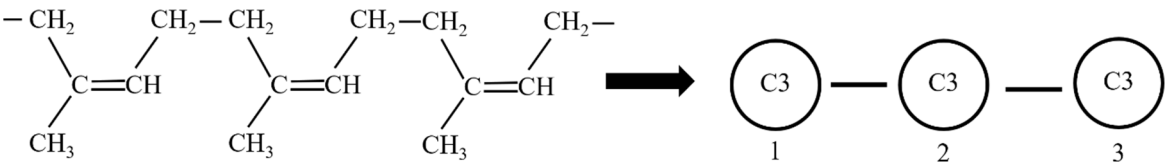
Rubber chain structure			
			
Bonded interaction		k_b (kJmol ⁻¹ nm ⁻²)	b_0 (nm)
1-2		5000	0.46
2-3		5000	0.46
Angle bending		k_θ (kJmol ⁻¹)	θ_0 (degree)
1-2-3		37	110
Non-bonded interaction: Lennard-Jones potential			
		C6	C12
C3	C3	0.15091	0.0016267

Table S2: Number of molecules and simulation time.

Fullerene Concentration (phr)	Number of Fullerene (molecule)	Number of <i>cis</i> -PI (chain)	Simulation time (μ s)
0	0	500	21
4	53	500	21
8	107	500	21
16	213	500	21
32	427	500	21

Table S3: Solvation free energy of an added fullerene in water, *cis*-PI in melt and composite at different C₆₀ concentrations.

Solvate	Free energy (kJ/mol)	Reference
Water	-99.53 \pm 0.03	-92.6 [1]
Melt	-215.08 \pm 0.14	
4phr	-214.37 \pm 0.10	
8phr	-213.95 \pm 0.29	
16phr	-212.40 \pm 0.13	
32phr	-210.43 \pm 0.33	

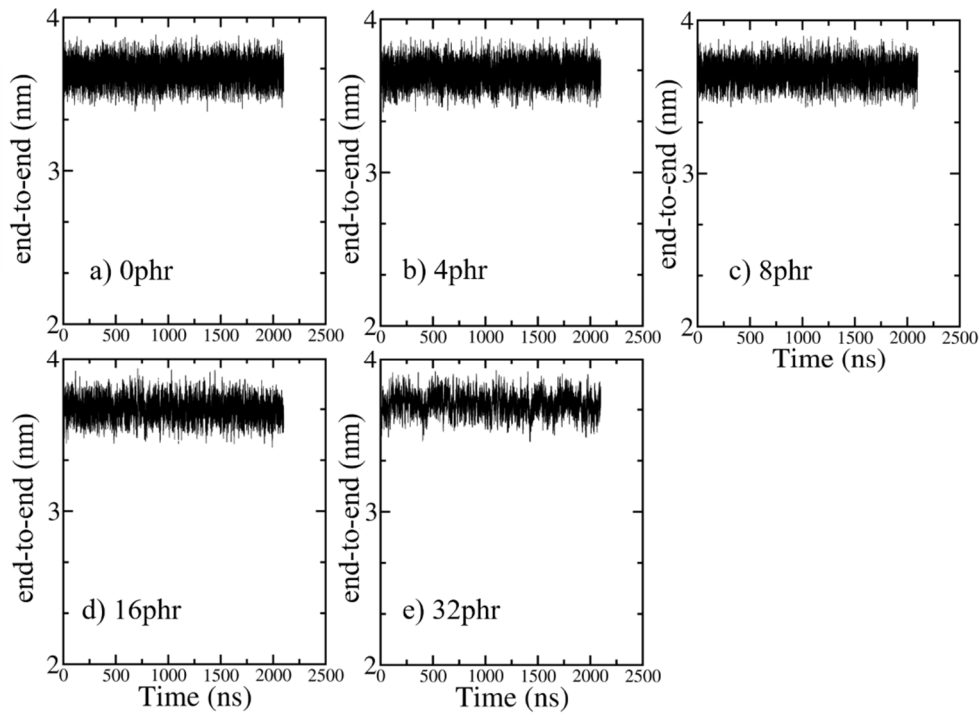


Figure S1: Time evolution of end-to-end distance (R_0) with varies C_{60} concentration from 0 to 32 phr.

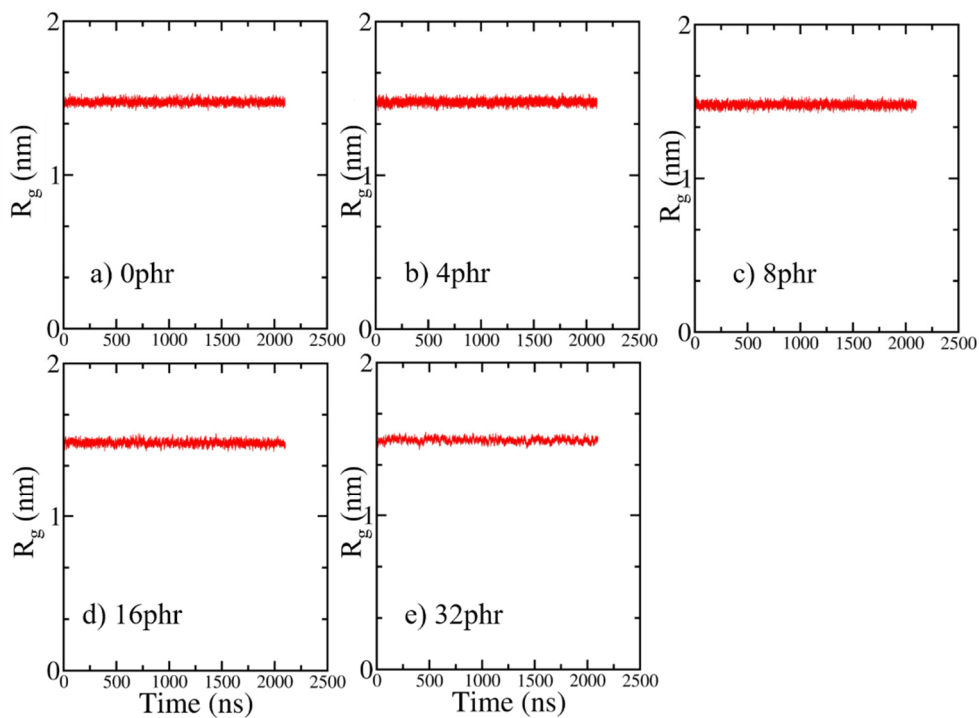


Figure S2: Time evolution of radius of gyration (R_g) with varies C_{60} concentration from 0 to 32 phr.

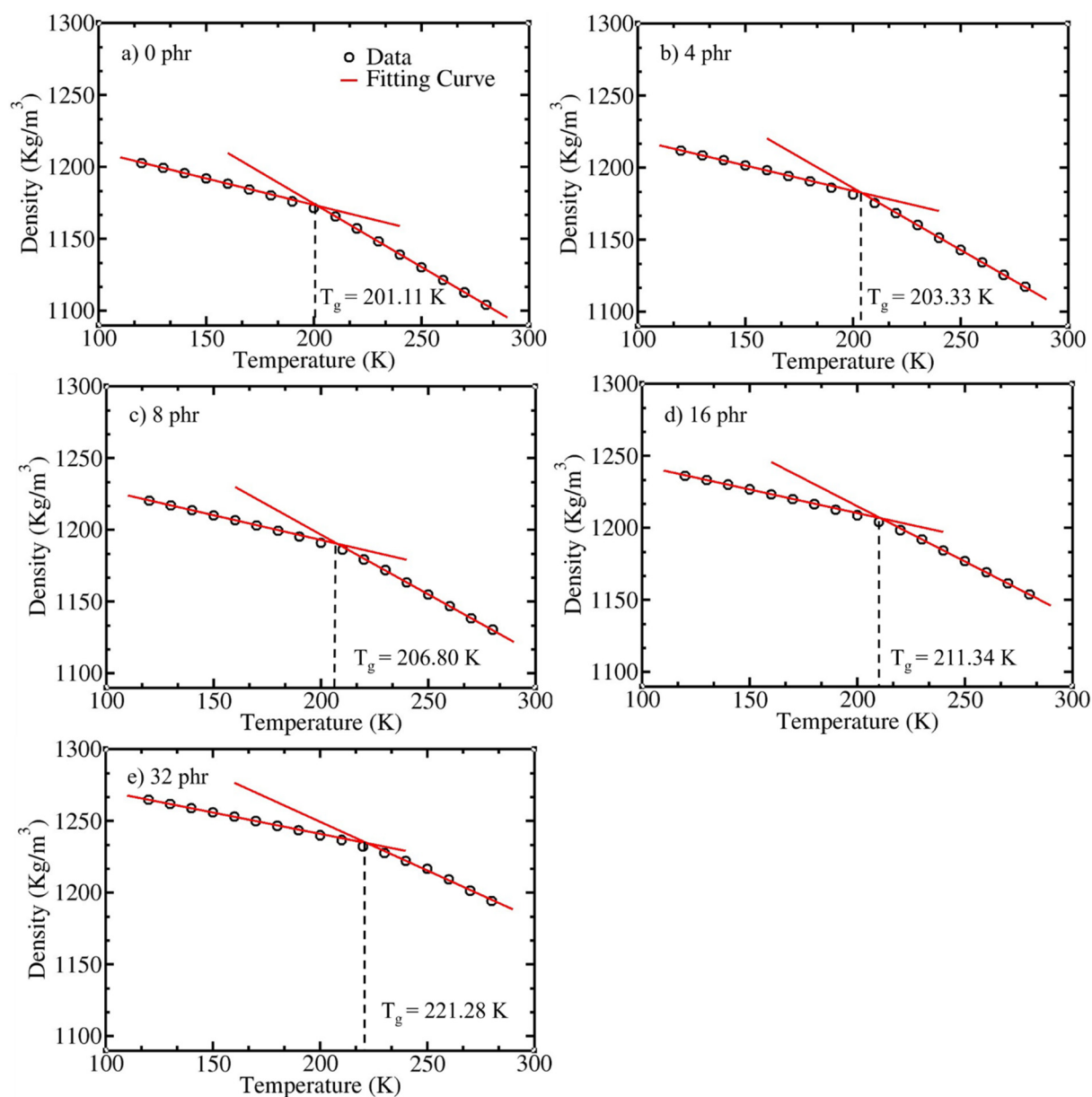


Figure S3: Density versus temperature of *cis*-PI-C₆₀ composites.

Reference

1. Nisoh, N.; Karttunen, M.; Monticelli, L.; Wong-Ekkabut, J. Lipid monolayer disruption caused by aggregated carbon nanoparticles. *RSC Adv.* **2015**, *5*, 11676-11685.