Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Structural and Dynamical Properties of Thermoplastic Polyurethane/Fullerene Nanocomposites: A Molecular Dynamics Simulations Study

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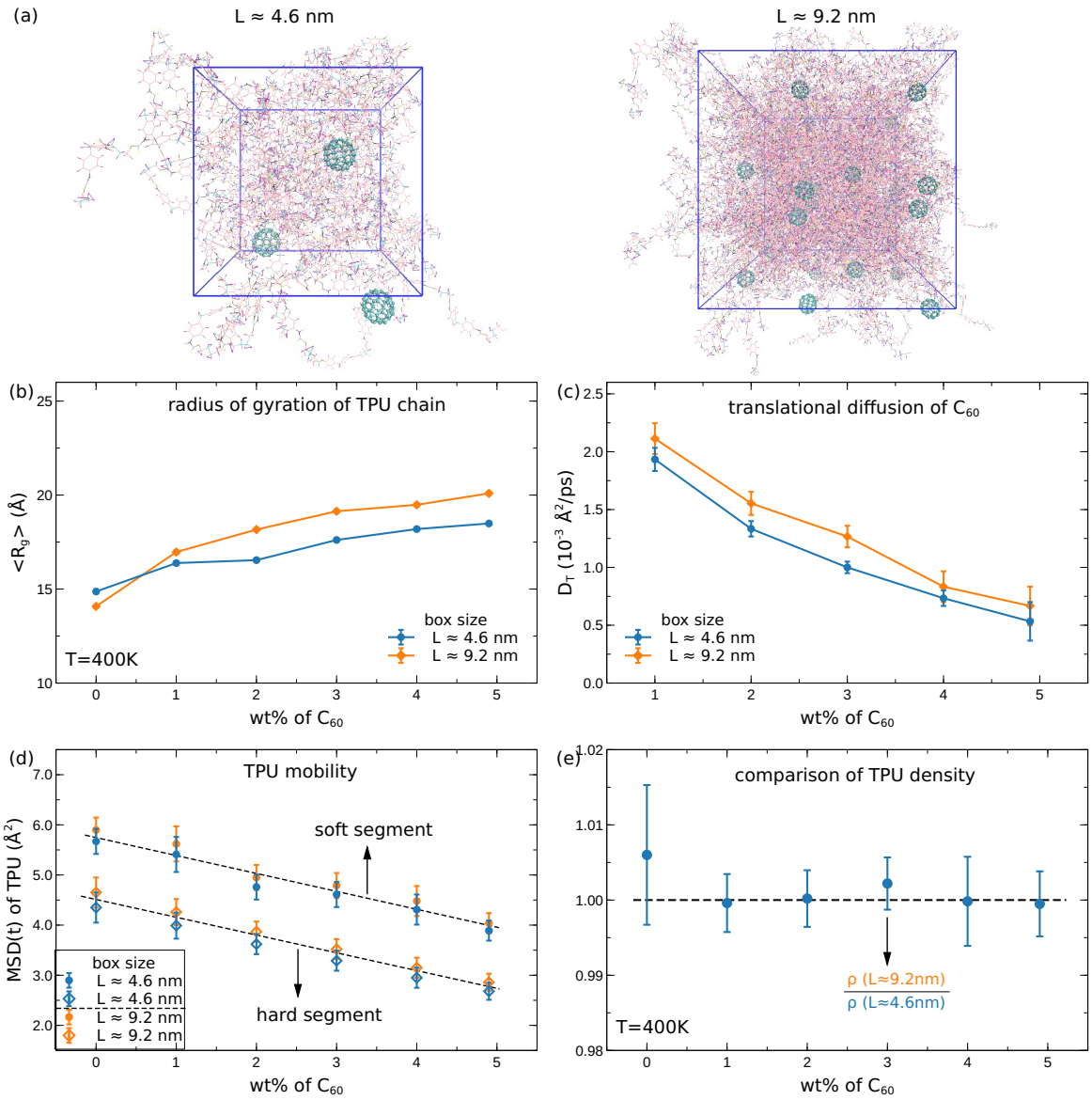

Figure S1: Finite size effect examined: (a) snapshots of simulation systems with smaller size ($L \approx 4.6nm$) and larger size ($L \approx 9.2nm$), (b) radius of gyration ($< R_g >$) as a function of C_{60} wt% for the smaller and larger simulation systems, (c) translational diffusion coefficient (D_{T}) as a function of C_{60} wt% influenced by simulation size, (d) MSD($t = 100ps$) of TPU for soft and hard segments with respect to C_{60} wt%, (e) The ratio of TPU density between the larger system ($L \approx 9.2nm$) and the smaller system ($L \approx 4.6nm$).

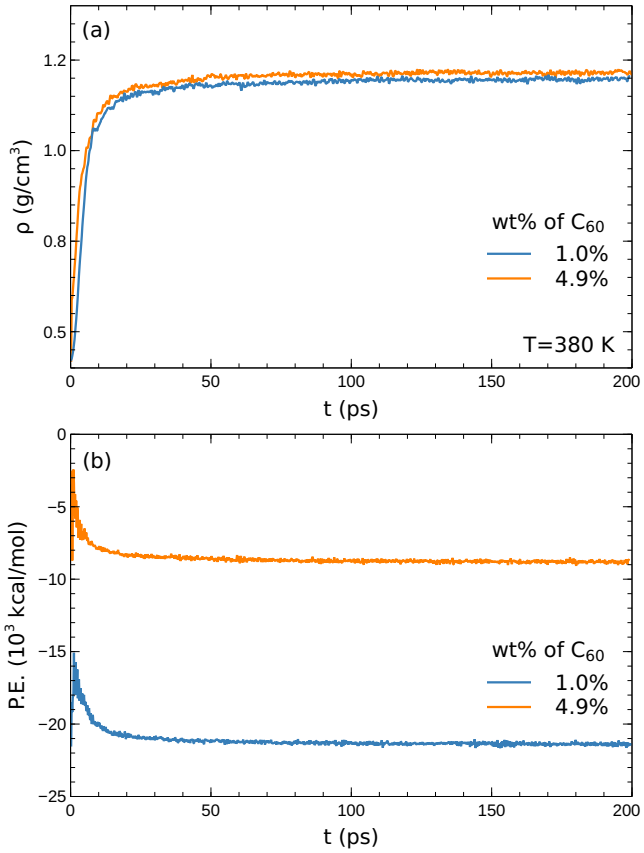

Figure S2: Changes in (a) density of TPU/C_{60} composites and (b) potential energy during the first 200 ps of NPT run (P=0.1 MPa, T=380 K).

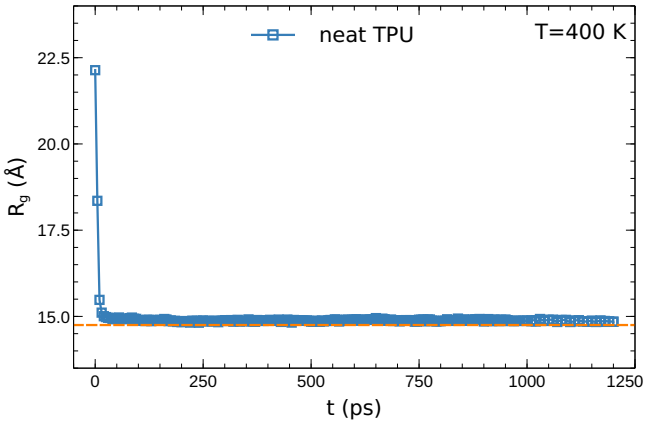

Figure S3: Radius of gyration (R_g) of TPU chain as a function of simulation time (P=0.1 MPa, T=400 K). The theoretical value of R_g is given by the dashed line.

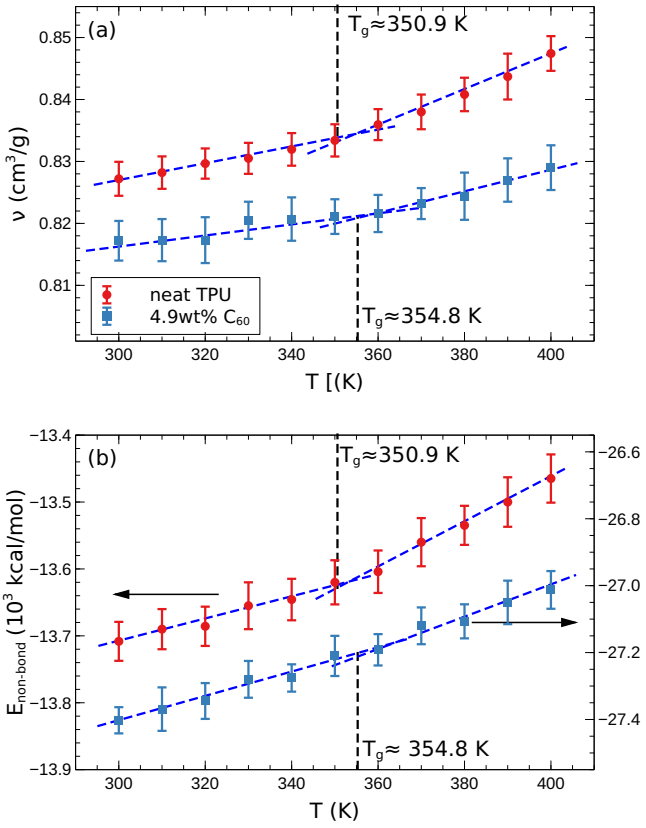

Figure S4: Determination of glass transition temperature T_g by changes in (a) specific volume (ν) and (b) non-bond energy ($E_{\text{non-bond}}$) versus temperature (T).

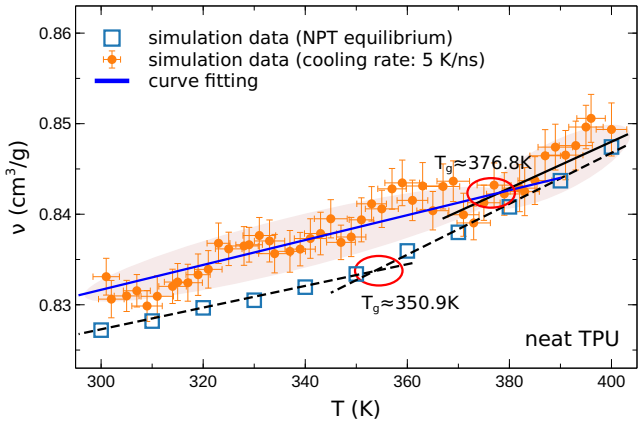

Figure S5: Specific volume (ν) under NPT equilibrium and during cooling, as a function of temperature (T). Glass transition temperature (T_g) measured using cooling is significantly higher compared to simulation technique of NPT equilibrium.

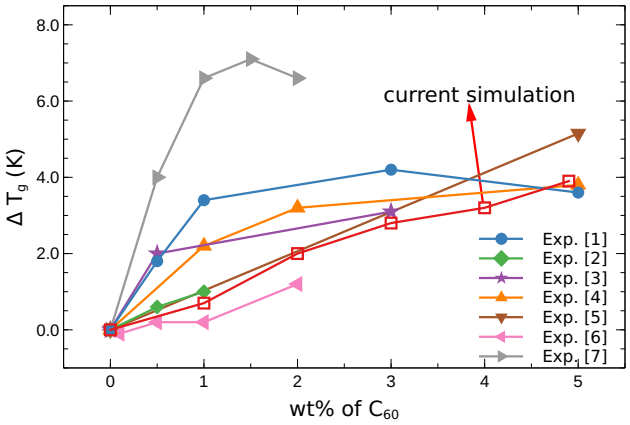

Figure S6: Comparison of glass transition temperature increment (ΔT_g) from current MD simulation study and literature experiments. Polymer/C_{60} composite details shown in Table S1.

Table S1: Polymer/C_{60} composite systems in literature experiments

Index	Polymer/C_{60} System[a]	Molecular Weight of Polymer	References
–	TPU/C_{60}	Mw=Mn=3494 g/mol	Current Simulation
Exp. [1]	PMMA/C_{60}	Mw=254.7 kg/mol	[1][1]
Exp. [2]	PS/C_{60}	Mw=152 kg/mol	[2][2]
Exp. [3]	PIB/C_{60}	Mn=25000 g/mol	[3][3]
Exp. [4]	PS/C_{60}	Mw=2.2 kg/mol	[4][4]
Exp. [5]	PS/C_{60}	Mn=2727 g/mol	[5][5]
Exp. [6]	PU/C_{60}	Mn=∼24000 g/mol	[6][6]
Exp. [7]	TPU/C_{60}	unknown	[7][7]

[a] polymer abbreviation: TPU - thermoplastic polyurethane; PMMA - poly(methyl methacrylate); PS – polystyrene; PIB – polyisoprene; PU – polyurethane;

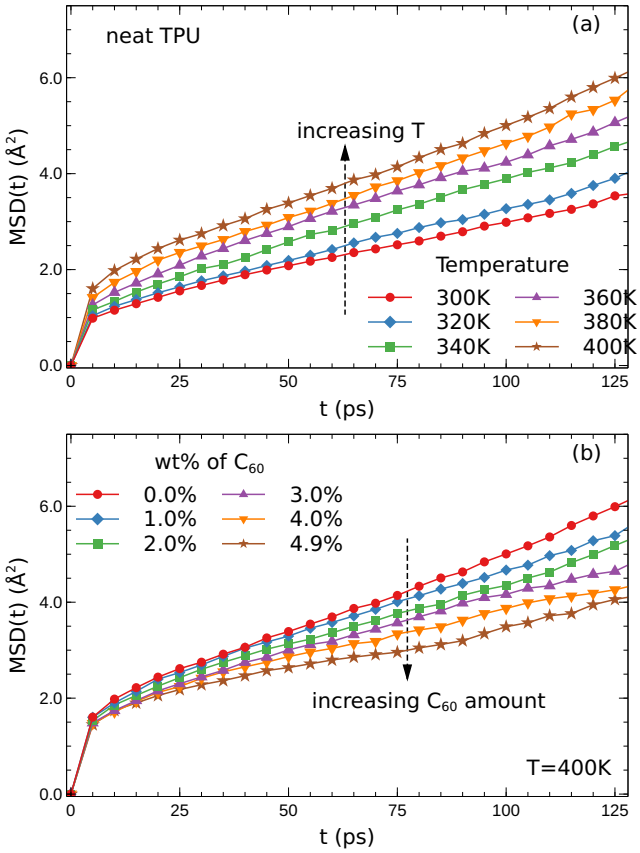

Figure S7: (a) Mean squared displacement (MSD(t)) versus time t for neat TPU. (b) MSD(t) for TPUs with varying wt% of C_{60} at 400K.

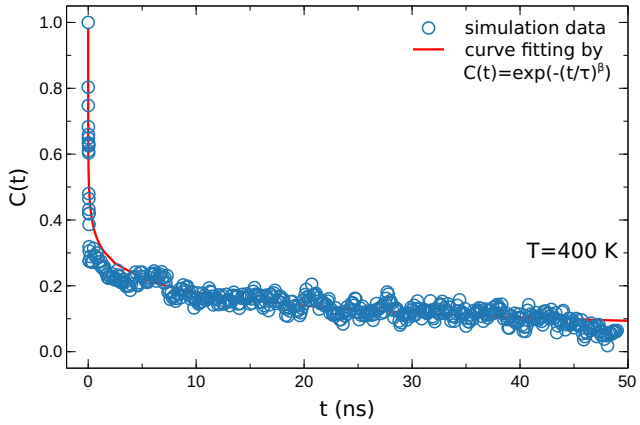

Figure S8: Time decay of orientational autocorrelation function $C(t)$ for bond vector of simulated TPU chains (P=0.1 MPa, T=400 K).

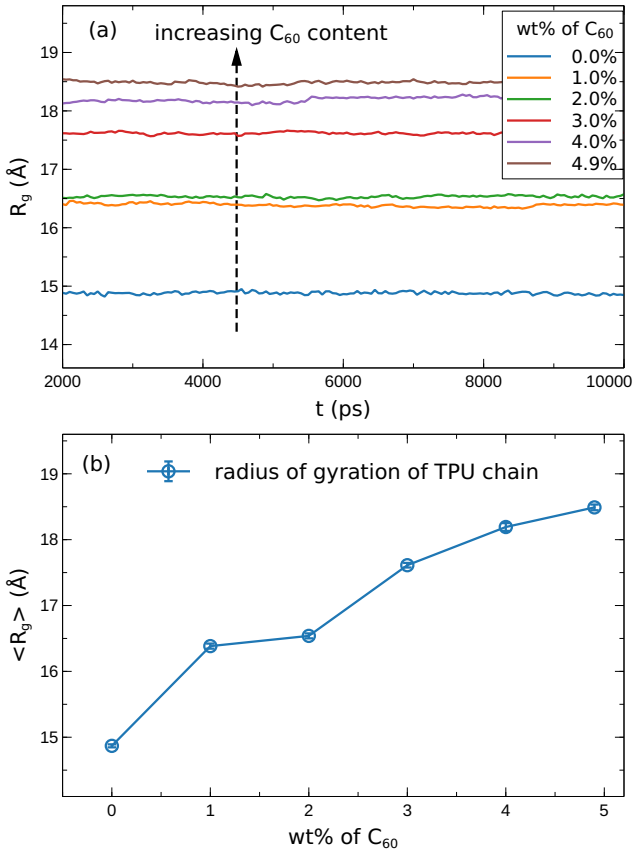

Figure S9: (a) Time dependence of radius of gyration (R_g) of TPU chains within intermediate to long-time range. (b) Averaged radius of gyration ($\langle R_g \rangle$) as a function of C_{60} wt%.

References

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