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Supporting Information

for

Characterization of the Structural, Mechanical, and Electronic Properties of Fullerene Mixtures: A Molecular Simulations Description

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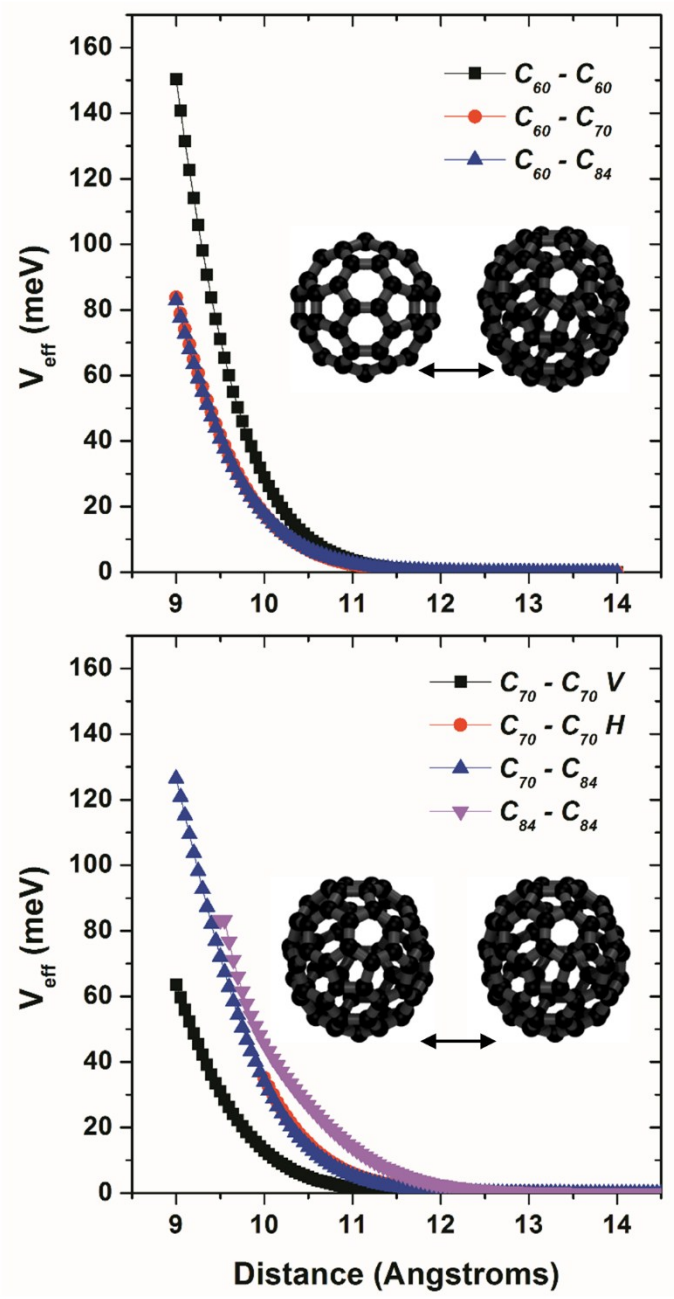

Figure S1: Exponential fits (data points are filled symbols) to the transfer integrals (calculated at the ωB97XD/6-31G(d,p) level of theory) between pairs of fullerenes as a function of distance between the centers-of-mass. Fullerene molecules are oriented such that the hexagonal faces on C_{60} and C_{70} are aligned and parallel to each other. Representative illustrations of the C_{60} - C_{70} pair (top-inset) and C_{70} - C_{70} pair (bottom-inset) are also shown.

Table S1: Parameters (V_0 and b) obtained from the fit of the transfer integrals (V_{eff}) to an exponential ($V_{eff} = V_0 e^{-bx}$) dependence on inter-molecular distance, x. Errors bars associated with the fitted parameters are given between parentheses.

System	$V_0/10^8$ (meV)	b (1/Å)
C_{60} - C_{60}	3.79 (0.49)	1.63 (0.01)
C_{60} - C_{70}	0.96 (0.14)	1.55 (0.01)
C_{60} - C_{84}	0.85 (0.09)	1.53 (0.01)
C_{70} - C_{70} (V)	1.0 (0.13)	1.58 (0.01)
C_{70} - C_{70} (H)	14.0 (1.14)	1.75 (0.01)
C_{70} - C_{84}	0.27 (0.04)	1.36 (0.02)
C_{84} - C_{84}	0.07 (0.01)	1.19 (0.01)

Table S2: Average polarization energy obtained from subtracting the SOMO eigenvalue of the isolated anion molecules (-2.14, -2.58, -3.13, -2.02, and -2.47 eV for C_{60}, C_{70}, C_{84}, $PC_{61}BM$, and $PC_{71}BM$, respectively) from the SOMO eigenvalues of the anionic clusters with the excess electron localized on the central molecule. In the anionic clusters, the first-neighbor shell of molecules is represented using atom-centered point charges. Computed error bars are 0.01-0.02 eV.

System	Mean Polarization Energy (eV)				
	C_{60}	C_{70}	C_{84}	$PC_{61}BM$	$PC_{71}BM$
C_{60}	0.54	-	-	-	-
C_{70}	-	0.64	-	-	-
$PC_{61}BM$	-	-	-	0.46	-
$PC_{71}BM$	-	-	-	-	0.36
C_{60}:C_{70} (0.95:0.05)	0.63	0.67	-	-	-
C_{60}:C_{70} (0.90:0.10)	0.64	0.65	-	-	-
C_{60}:C_{70}:C_{84} (0.95:0.045:0.005)	0.60	0.63	0.61	-	-
C_{60}:C_{70}:C_{84} (0.90:0.09:0.01)	0.63	0.65	0.62	-	-
$PC_{61}BM$:$PC_{71}BM$ (0.95:0.05)	-	-	-	0.49	0.28
$PC_{61}BM$:$PC_{71}BM$ (0.90:0.10)	-	-	-	0.49	0.31

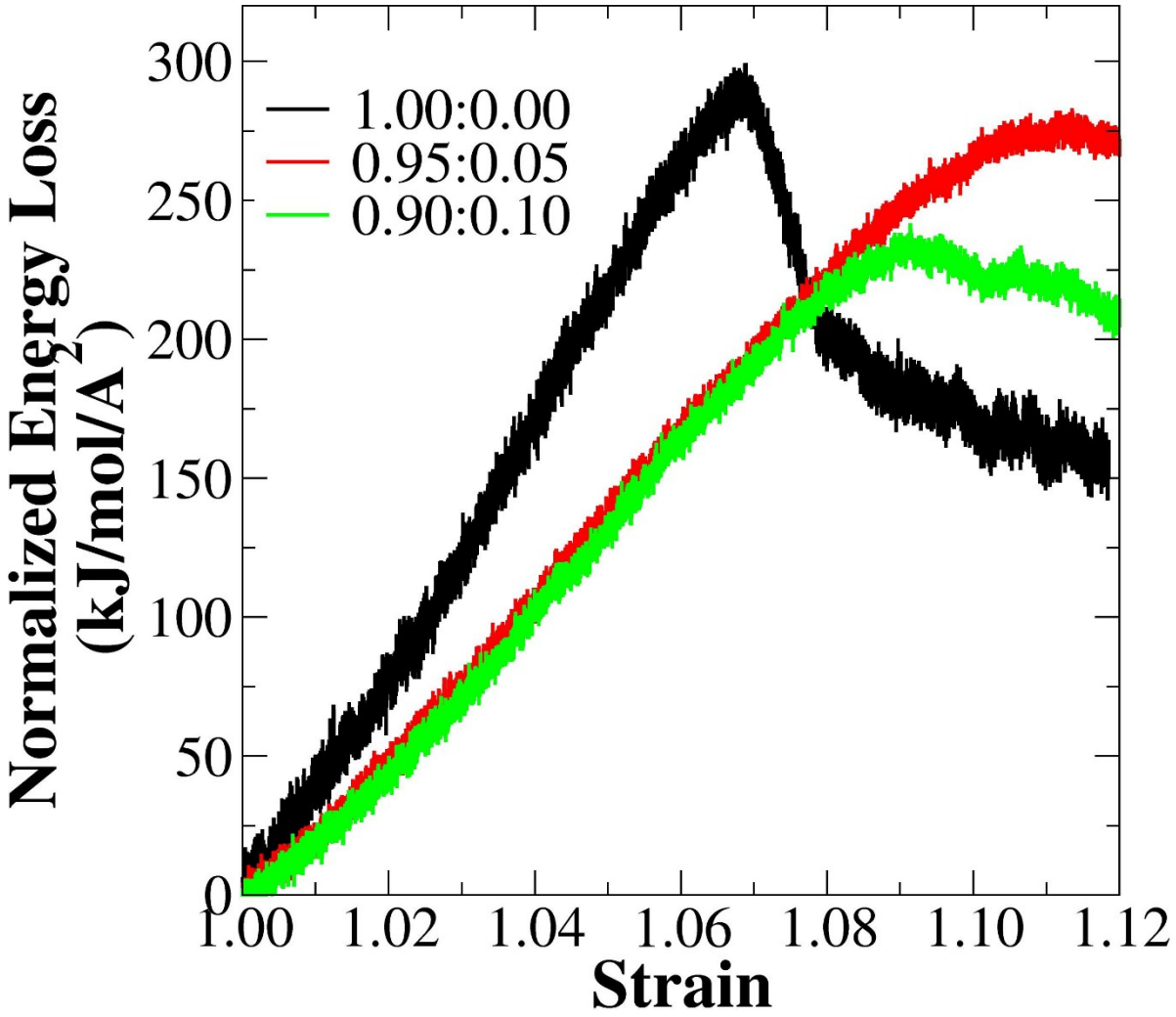

Figure S2: Short-range Lennard-Jones energy loss due to the expansion of the simulation box for pure $PC_{61}BM$ and $PC_{61}BM$:$PC_{71}BM$ mixtures. Strain is defined as the ratio of increase in length of simulation box upon expansion over the initial length of the simulation box in the direction of elongation. As the system expands, loss of intermolecular interactions continues until the film breaks, after which the molecules in the two separate parts rearrange to reach eventually the density of the corresponding amorphous packing; hence, the gain in interaction energy.