

Influence of Ionic Liquids on the Chain Dynamics and Enthalpy Relaxation of Poly(methyl methacrylate)

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SUPPORTING

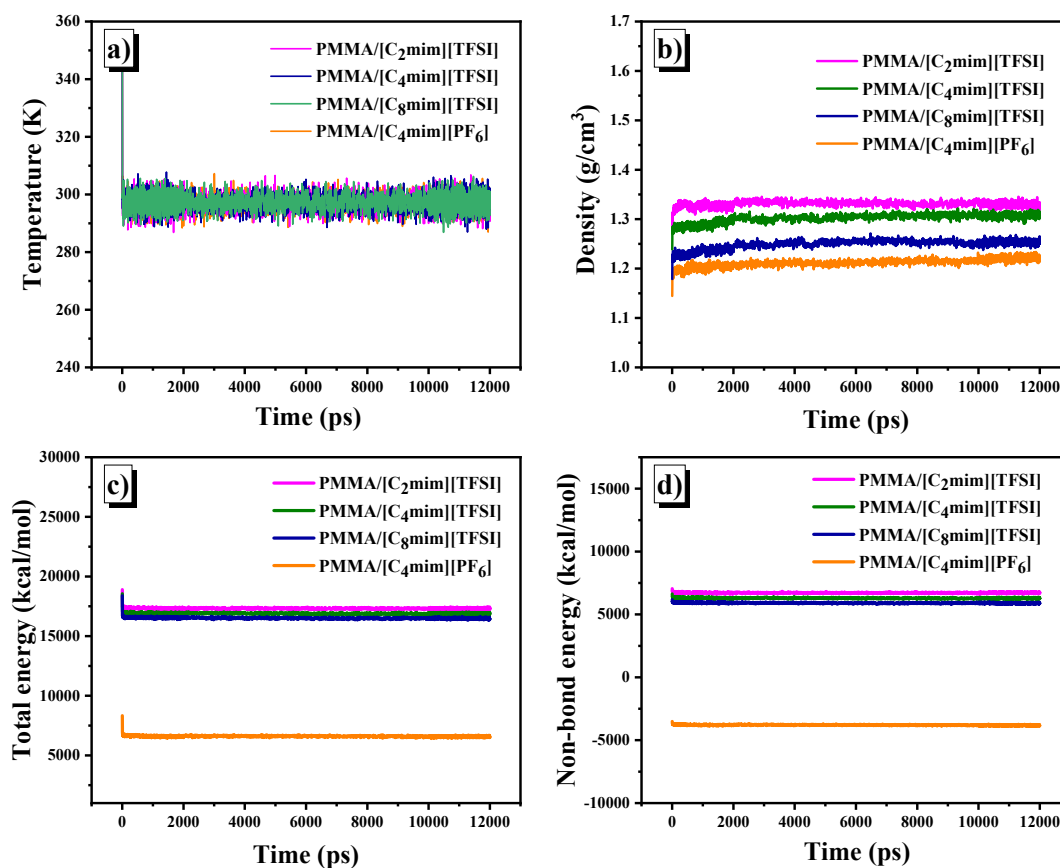


Figure. S1 The related parameters in molecular dynamic simulations (NPT ensembles) for PMMA/ILs blends (at the weight ratio of 50:50): temperature a), density b), total energy c) and non-bond energy d).

Table. S1 Comparison of density between reference and our simulation result. Where physicochemical properties of ILs was referred to Watanabe's work (H. Tokuda, S. Tsuzuki, M. A. B. H. Susan, K. Hayamizu and M. Watanabe, *J. Phys. Chem. B*, 2006, **110**, 19593-19600).

ILs	ρ (g/cm ³) at 25 °C ^a	ρ (g/cm ³) at 298 K ^b (our NPT)	Std. Dev.
[C ₂ mim][TFSI]	1.519	1.64	8.0%
[C ₄ mim][TFSI]	1.437	1.55	7.9%
[C ₈ mim][TFSI]	1.320	1.40	6.1%
[C ₄ mim][PF ₆]	1.368	1.41	3.1%

Table. S2 Related parameters in molecular dynamic simulations for cohesive energy density (CED) and χ calculation.

Force field: COMPASS II	[C ₂ mim][TFSI] +PMMA	[C ₄ mim][TFSI] +PMMA	[C ₈ mim][TFSI] +PMMA	[C ₄ mim][PF ₆] +PMMA
CED _{blends} (J/cm ³)	1064.7	1005.6	891.6	1253.0
CED _{IL} (J/cm ³)	2179.9	1972.4	1613.8	2496.6
CED _{PMMA} (J/cm ³)	246.1	246.1	246.1	246.1
φ_{IL}	0.422352	0.432998	0.462893	0.449071
φ_{PMMA}	0.577648	0.567002	0.537107	0.550929
$\varphi^*CED(IL)$	920.6851	854.0444	747.0172	1121.152
$\varphi^*CED(PMMA)$	142.1592	139.5393	132.182	135.5835
ΔE_{mix} (J/cm ³)	-1.85574	-12.0163	-12.4008	3.735397
V_m (cm ³ /mol)	257	292	360	207.6
χ	-0.1925	-1.4162	-1.80188	0.312995

Table. S3 PALS related parameters.

PMMA/ILs 70/30 wt%	I_1 (%) ^d	I_2 (%) ^d	I_3 (%) ^d	T_g (°C)
[C ₂ mim][TFSI]	48.93	42.93	8.139	61.7
[C ₄ mim][TFSI]	50.25	41.49	8.263	59.6
[C ₈ mim][TFSI]	50.25	40.54	9.208	54.2
[C ₄ mim][PF ₆]	51.02	40.56	8.425	61.8

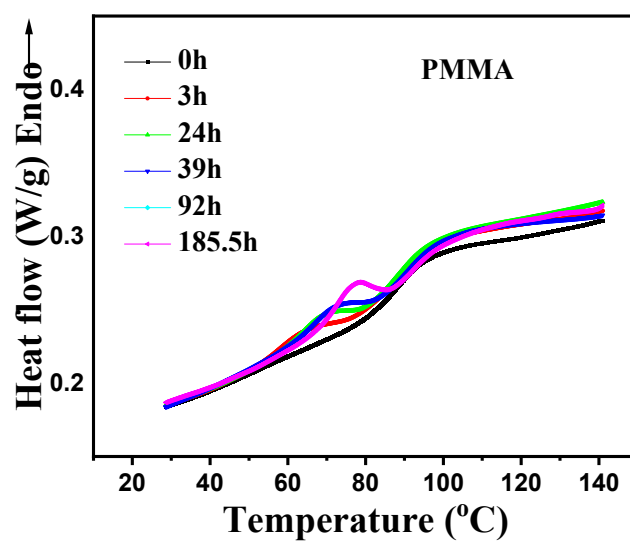


Figure. S2 DSC heating scan curves for PMMA aged at 50 °C for different time.