Electronic Supplementary Material (ESI) for Soft Matter

A Molecular investigation of nanostructure and dynamics of Phosphoric/Triflic acid blends of hydrated ABPBI [poly(2,5-benzimidazole)] Polymer Electrolyte Membrane

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Supporting Information:

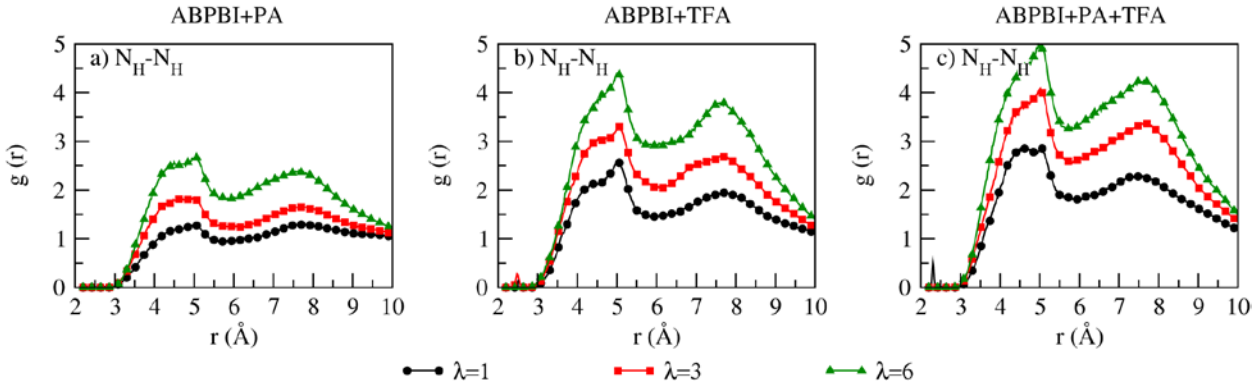

Figure S1: N_H-N_H RDFs from a) ABPBI+PA blends, b) ABPBI+TFA blends and c) ABPBI+PA+TFA blends.

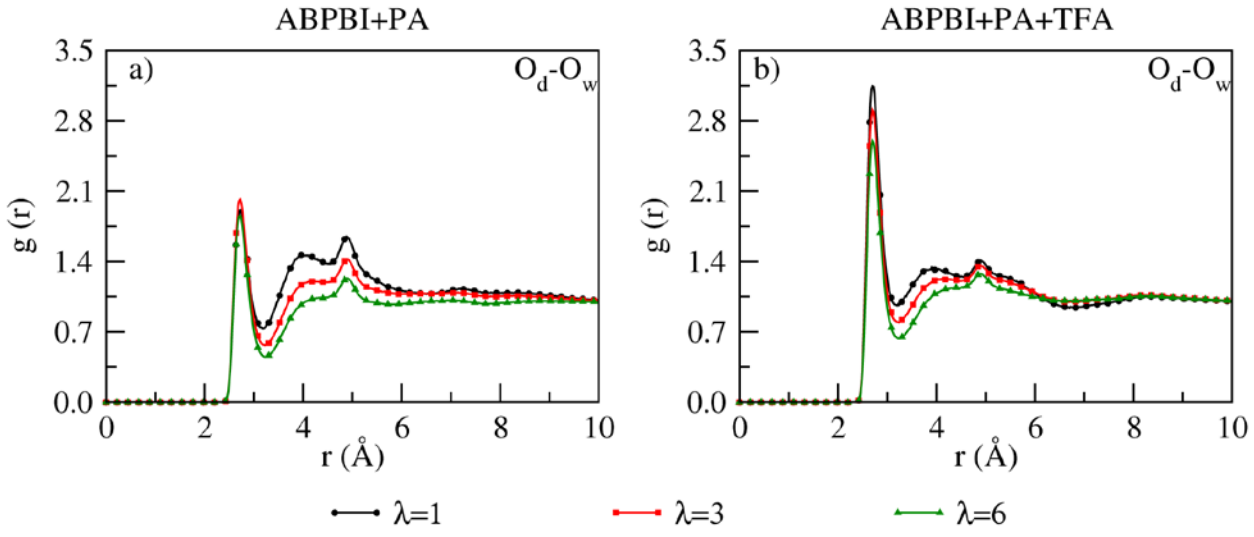

Figure S2: O_d-O_w RDFs from a) ABPBI+PA blends and b) ABPBI+PA+TFA blends.

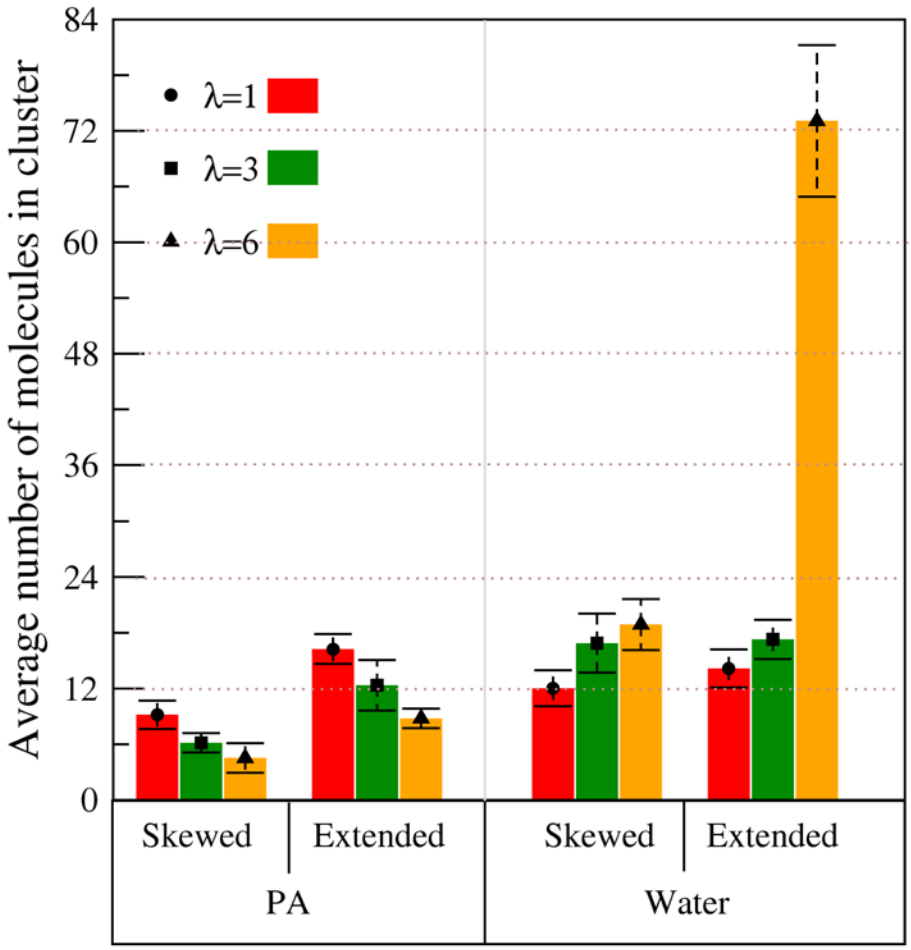

Figure S3: Average number of PA and water molecules in a cluster from ABPBI+PA blends. [Error bar represents standard deviation]

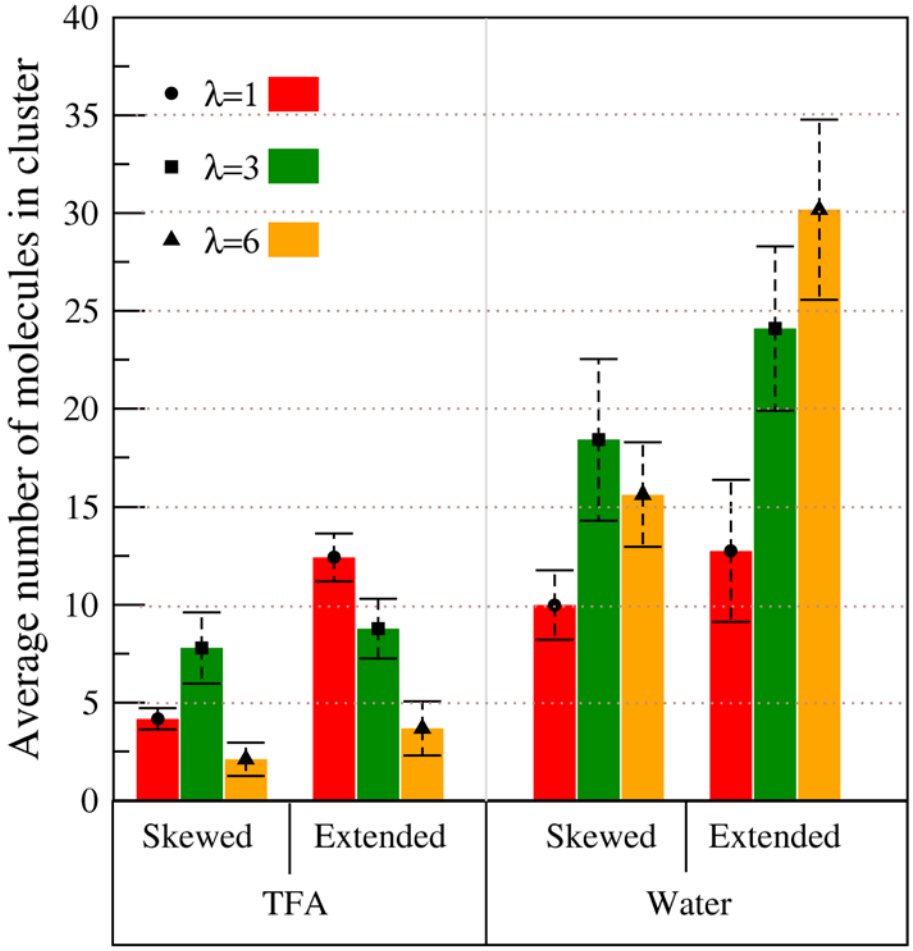

Figure S4: Average number of TFA and water molecules in a cluster from ABPBI+TFA blends. [Error bar represents standard deviation]

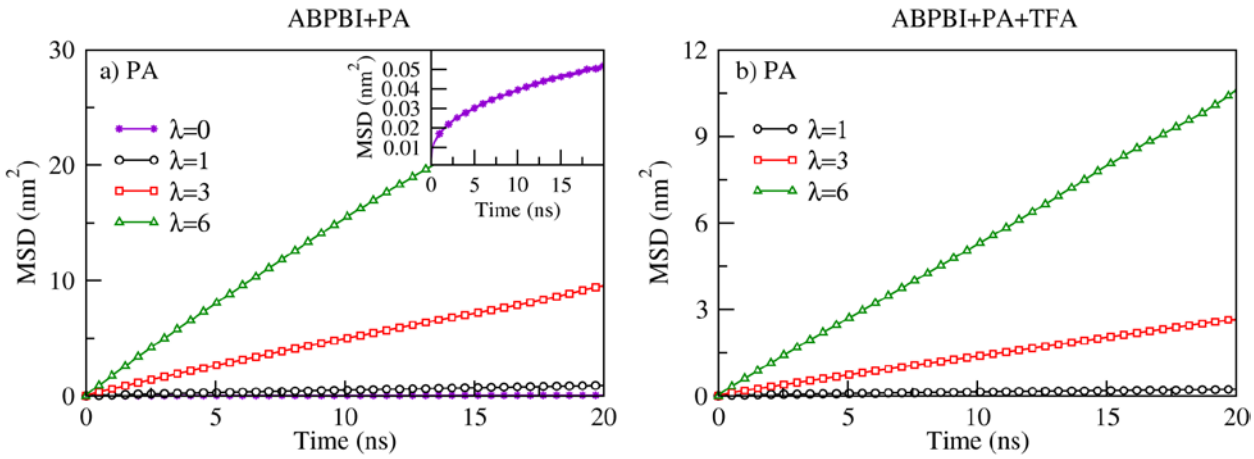

Figure S5: Mean Square Displacement of PA.

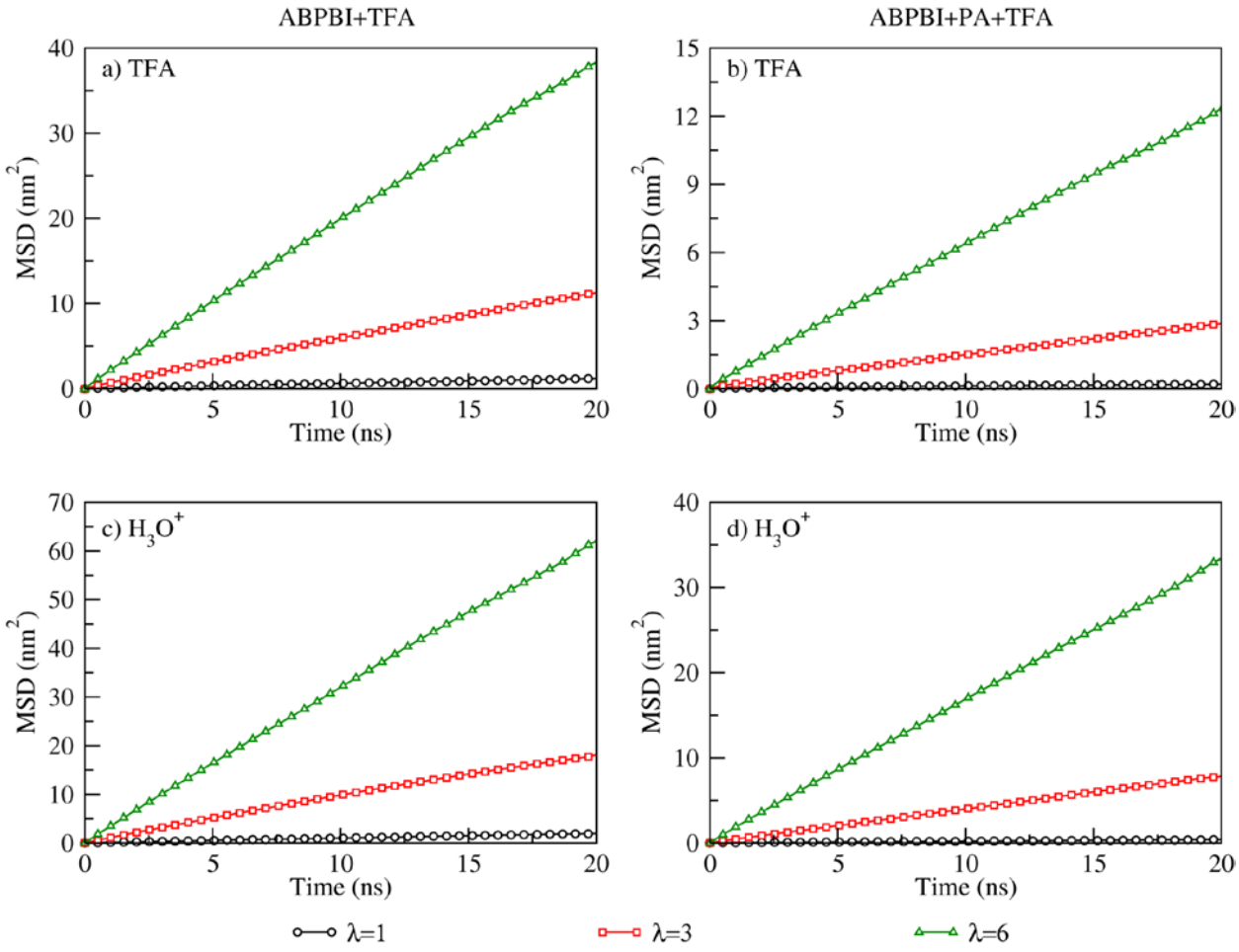

Figure S6: Mean Square Displacement of (a, b) TFA and (c, d) hydronium ions.

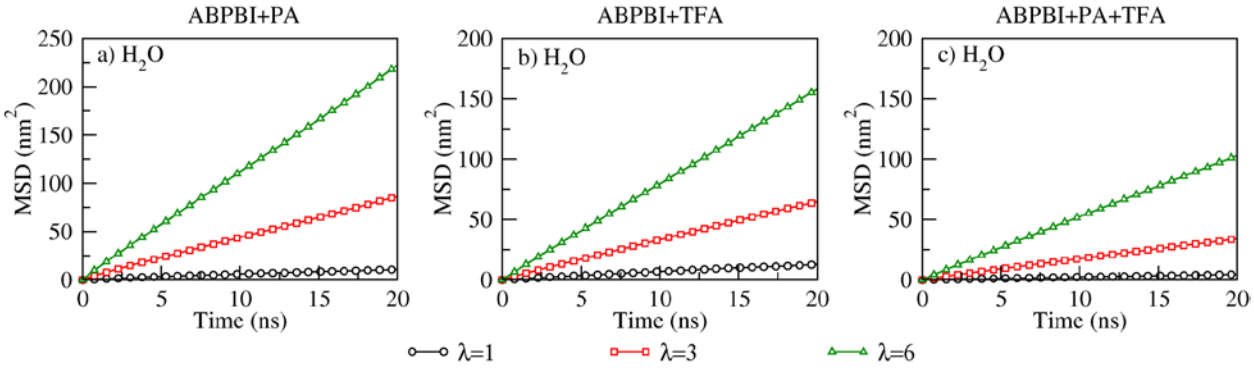

Figure S7: Mean Square Displacement of water molecules.

Table S1: Box length (Å), average density (g cm^{-3}), end-to-end polymer chain distance (R_{E-E}), radius of gyration (Rg) and Diffusion coefficients ($D_A \times 10^{-5}$ cm^2 sec^{-1}) of PA, hydronium ions, TFA and water molecules in hydrated (λ=3) ABPBI+PA+TFA blend.

System	[ABPBI + PA + TFA][a]	[ABPBI + PA + TFA][b]
Total No. of atoms	45568	91008
No. of PA molecules	1280	2560
No. of TFA molecules	1280	2560
No. of water molecules	3840	7680
Box length (Å)	80.5541	101.6332
Density (g cm^{-3})	1.5369 ± 0.0022	1.5301 ± 0.0022
R_{E-E} (Å)	29.1042 ± 11.2577	20.2490 ± 9.2409
Rg (Å)	11.8469 ± 1.9312	11.9717 ± 1.2403
R_{E-E}/Rg	2.45	1.69
D_A of PA	0.0217 ± 0.0002	0.0191 ± 0.0008
D_A of hydronium ions	0.0655 ± 0.0001	0.0767 ± 0.0005
D_A of TFA	0.0232 ± 0.0002	0.0267 ± 0.0017
D_A of water	0.2792 ± 0.0085	0.3098 ± 0.0133
[a](polymer chain from 10 monomers: i.e. n=10), [b](polymer chain from 20 monomers: i.e. n=20)		

Table S2: Co-ordination number calculated using the first minima (in parenthesis) from interactions in hydrated (λ=3) ABPBI+PA+TFA blend.

Polymer chain length	N-N (5.8 Å)	N-N_H (3.6 Å)	N-H_N (3.2 Å)	H_N-O_w (2.6 Å)
n=10	2.56	0.41	0.41	0.22
n=20	2.60	0.39	0.39	0.24

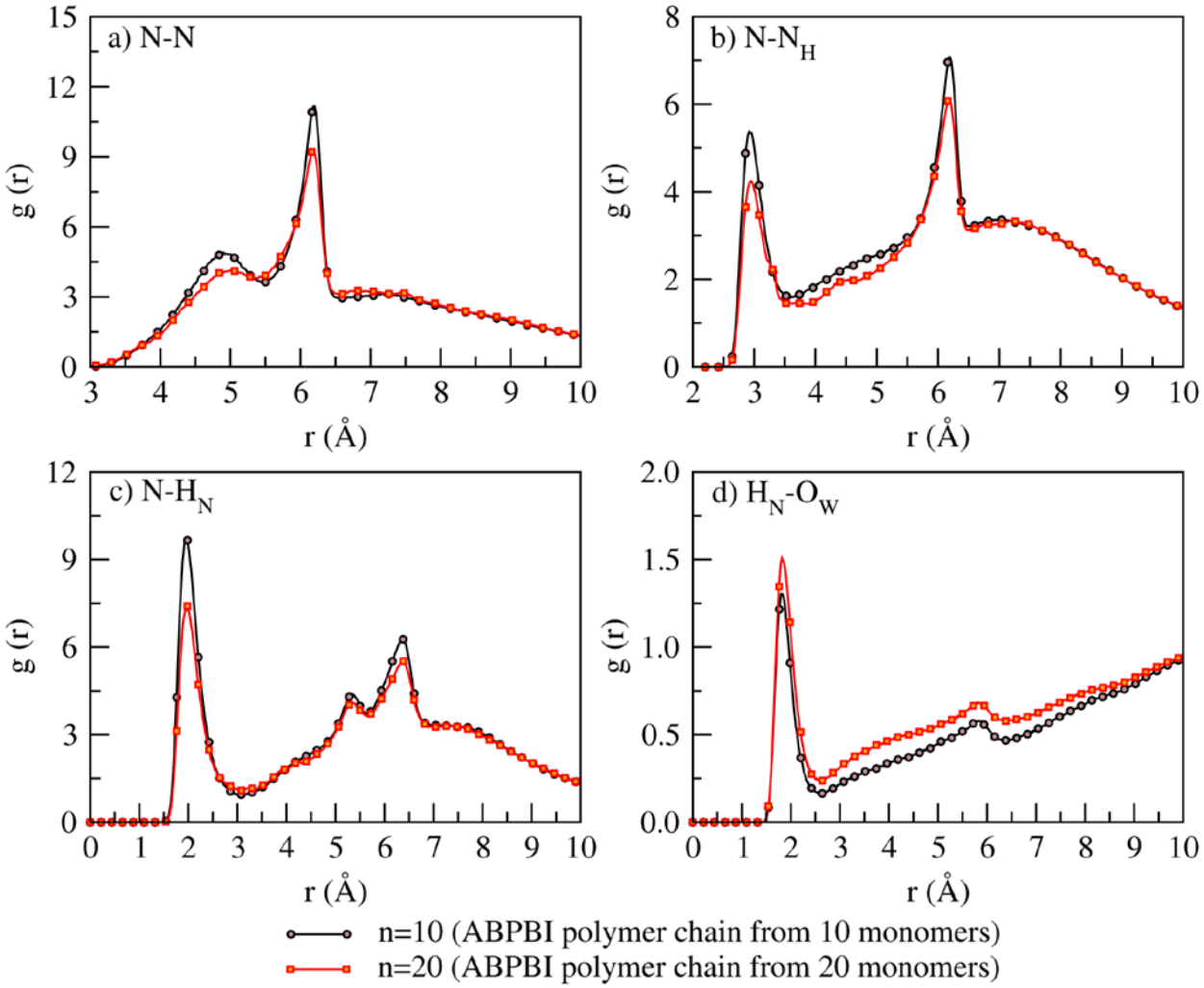

Figure S8: RDFs of a) N-N, b) N-N_H, c) N-H_N and d) H_N-O_w in hydrated (λ=3) ABPBI+PA+TFA blend.

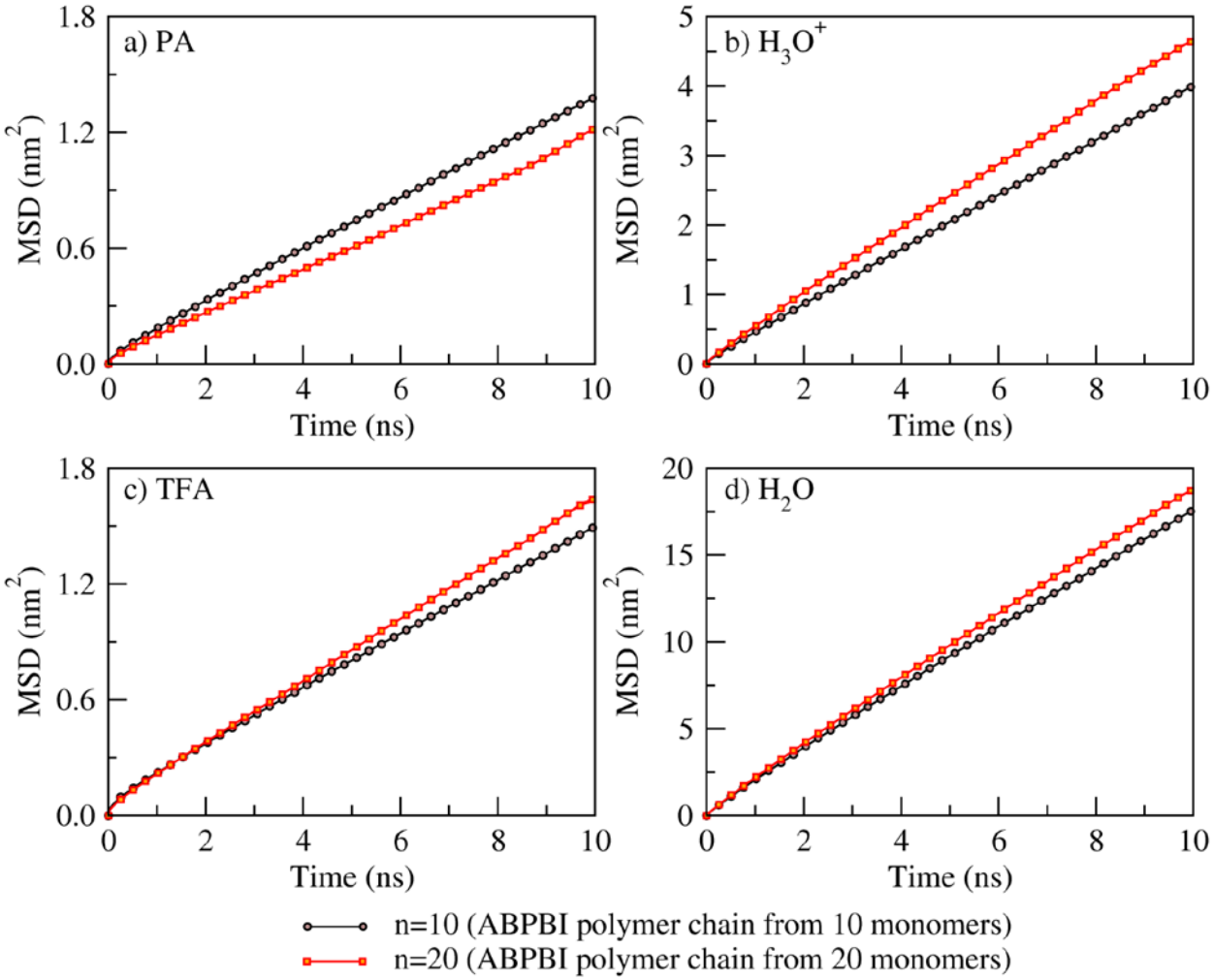

Figure S9: Mean Square Displacement of (a) PA, (b) hydronium ions, c) TFA, and (d) water from hydrated (λ=3) ABPBI+PA+TFA blend.