Supporting information for: Role of Salt and Water in the Plasticization of PDAC/PSS Polyelectrolyte Assemblies

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Supporting information datasets as figures

Figure S1 presents the pure water diffusion coefficient D_0 calculated following the NPT setup detailed in the main article for TIP4P water.[1] The system size is 2500 water molecules and the simulation box is approximately cubic. Figure S2 shows the mean square displacement (MSD) of (a) PDAC and (b) PSS molecules in the molecular dynamics simulations as a function of simulation time for simulated systems with salt molar ratio of $x = 1.5$. Above

the expected thermal transition temperature T_{tr}, the MSD data sets have modestly sparser spacing in the graphs.

Figure S3 shows the number density distribution functions of the water molecule contacts with the salt ions at different temperatures at salt molar ratio $x = 1.0$. The number density distributions are expressed as $\rho g(r)$, where ρ is the global number density and $g(r)$ the radial distribution function (RDF) of the corresponding atom pair.

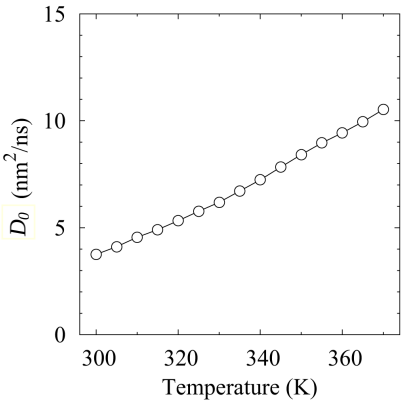

Figure S1: Pure water diffusion coefficient D_0 at different temperatures. The employed water model is TIP4P [1] and the calculation is done in a cubic simulation box containing 2500 water molecules.

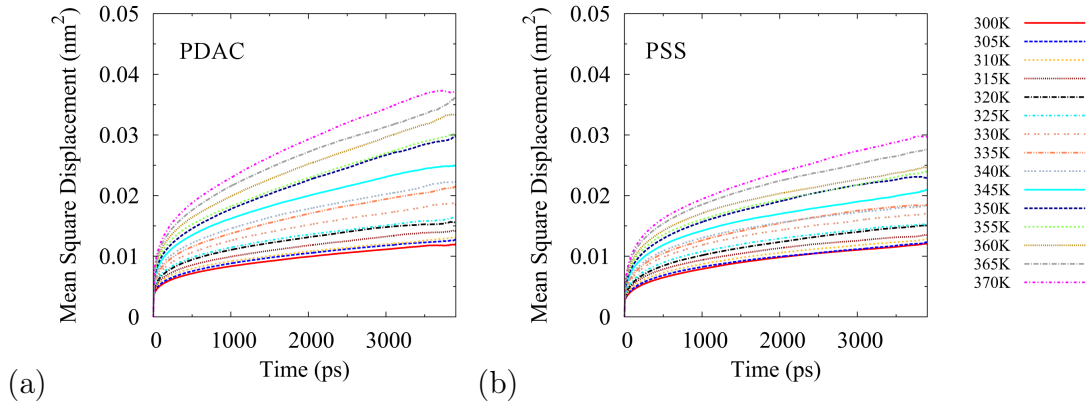

Figure S2: Mean square displacement (MSD) of (a) PDAC and (b) PSS molecules at salt molar ratio of $x = 1.5$ at different temperatures between 300 K and 370 K.

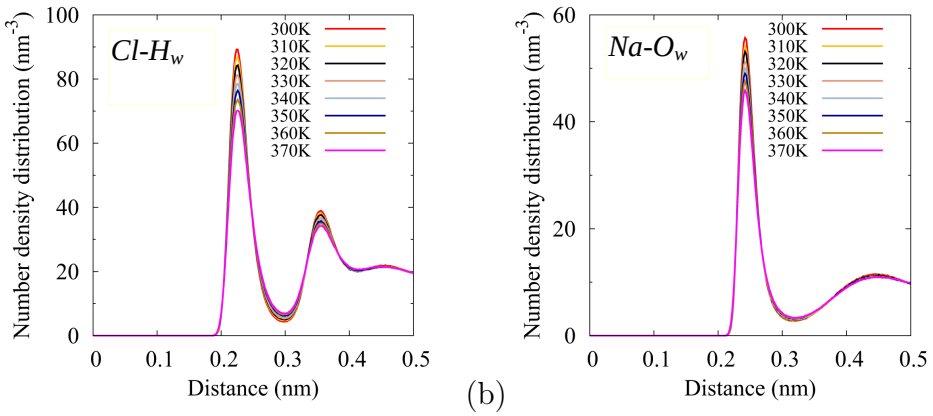

Figure S3: Number density distribution functions of (a) Cl-H_w and (b) Na-O_w contacts at different temperatures expressed as $\rho g(r)$, where ρ is the global number density and $g(r)$ the radial distribution function (RDF) of the corresponding atom pair. Here H_w and O_w are the water hydrogen and oxygen, respectively. The salt molar ratio $x = 1.0$.

References

(1) Jorgensen, W. L.; Chandrasekhar, J.; Madura, J. D.; Impey, R. W.; Klein, M. L. Comparison of Simple Potential Functions for Simulating Liquid Water. *J. Chem. Phys.* **1983**, *79*, 926–935.