Electronic Supplementary Material (ESI) for Soft Matter

Atomistic Simulations of Structure and Dynamics of Hydrated Aciplex Polymer Electrolyte Membrane

*Anurag Prakash Sunda and Arun Venkatnathan**

Supporting Information:

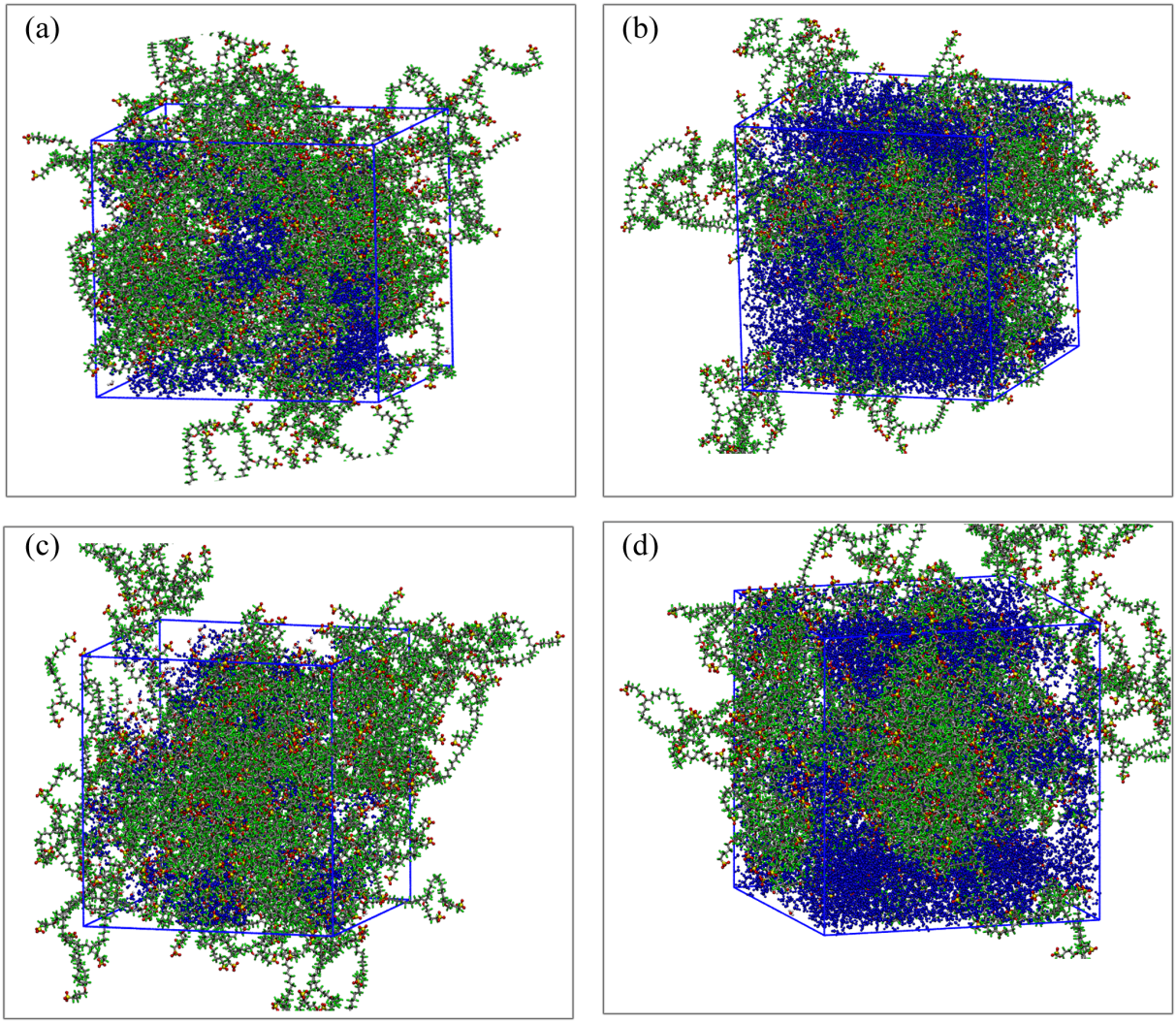

Figure S1: Snapshots of Aciplex ionomer membrane/water mixtures at 300 K (a, b) Initial configuration of randomly inserted water molecules in membrane matrix at λ=3 and λ=15 respectively; (c, d) Final configuration of production run at λ=3 and λ= 15 respectively.

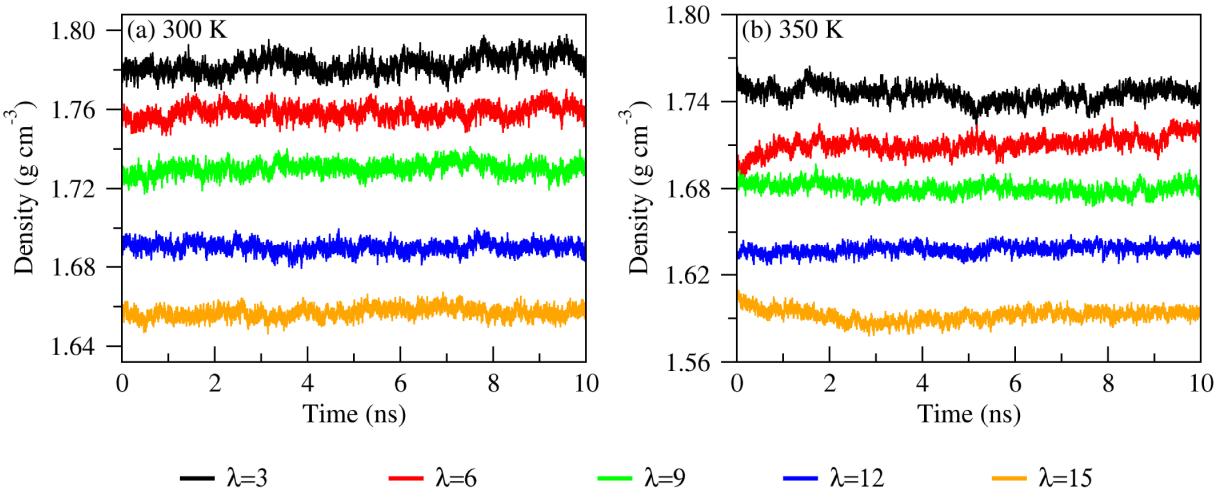

Figure S2: Density of Aciplex ionomer membrane/water mixtures at a) 300 K and b) 350 K.

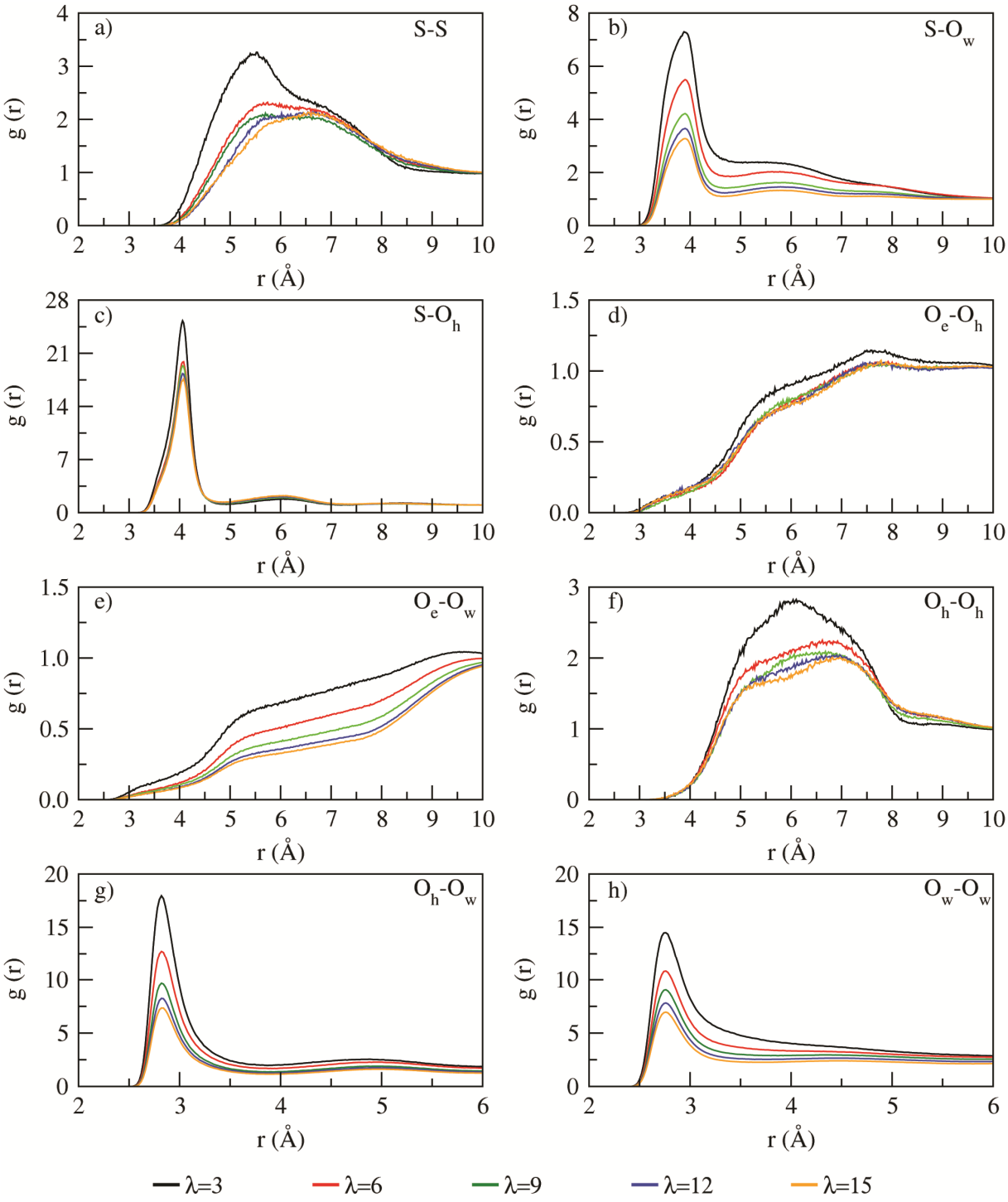

Figure S3: Radial distribution functions of a) S-S, b) S-O_w, c) S-O_h, d) O_e-O_h, e) O_e-O_w, f) O_h-O_h, g) O_h-O_w and h) O_w-O_w at 350 K.